

Simulation and Multi-objective Optimization of Vacuum Ethanol Fermentation

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Abstract: With the overall objective of optimizing an integrated first and second generation bioethanol production plant, a simple illustrative example is first used to examine the advantages and challenges of using a combination of VBA and UniSim Design for multi-objective optimization. In this paper, the simulation and optimization of a vacuum fermentation system using glucose and xylose as substrates is performed. The simulation of the fermentation system and the optimization are performed in the VBA environment, while UniSim Design is used to provide thermodynamic data necessary to perform calculations and used to simulate the downstream portion of the fermentation vacuum system. The Pareto domain of the system was circumscribed based on three decision variables (starting time of vacuum, rate of broth removal by vacuum and condenser temperature) and four objective functions (minimum ethanol loss, maximum productivity, minimum residual sugars and minimum compression energy). The procedure developed has allowed to easily circumscribe the Pareto domain of this system and to observe clearly the compromises that are required when all objective functions are optimized simultaneously. Some challenges to overcome are the time required for exchanging information between VBA and UniSim Design and the risk of non-converging for complex problems. For this procedure to be implemented effectively for the integrated ethanol plant, some innovative measures need to be developed.

1 INTRODUCTION

As a mean of partially reducing the world dependence on non-renewable petroleum as a fuel source and overall carbon dioxide emissions, research on biofuels has intensified significantly during the last decade with the main focus placed on bioethanol and biodiesel, and more recently on biobutanol. In many industrialized countries, over two thirds of the refined petroleum products sold is used for transportation purposes (NRCAN, 2009; U.S. EIA, 2010). This includes gasoline, low-sulphur diesel, and aviation fuel. There is therefore a need for a transitional fuel that will allow for a smooth changeover.

Bioethanol has great potential and has already been blended with some mainstream fuel sources at concentrations varying from 10% per volume up to

100%. Bioethanol has many advantages, including reduced dependence on imported oil, new markets for farmers and foresters, and a reduction of greenhouse gas (GHG) emissions from vehicles. Facing with the highly-publicized criticism of diverting farmlands or crops away from the human food chain supply (not the case for sugarcane), a shift to second-generation biofuels and a greater use of residual lignocellulosic biomass to produce biofuels is well underway to partly reduce this controversy.

The step before fermentation, to obtain fermentable sugars, and the microorganisms used in fermentation are the main differences between the ethanol production processes from simple sugar, starch or lignocellulosic material (Mussatto et al., 2010). The production of bioethanol from lignocellulosic biomass is significantly more

condenser in lieu of having a separate absorption column.

2.1 Fermentation Model

There are numerous models for predicting the production and consumption of the main species involved in fermentation. In this investigation, the model of Leksawasdi et al. (2001) was used. This model was developed for the batch fermentation of mixtures of glucose and xylose by recombinant *Zymomonas mobilis* strain ZM4(pZB5), containing additional genes for xylose assimilation and metabolism. The model represented very well experimental biomass growth, utilization of the two substrates and ethanol production over a large range of substrate concentrations.

This model has been adopted in this investigation to evaluate the in situ product recovery during fermentation operating at 30°C. The microbial growth on each sugar is modelled using Equation (1) with index j being 1 for glucose and 2 for xylose, respectively. This equation includes three terms affecting the maximum growth rate: (1) Monod kinetics for substrate limitation, (2) ethanol inhibition with a threshold level and a maximum inhibitory concentration, and (3) a typical substrate inhibition term.

$$r_{X,j} = \mu_{\max,j} \left(\frac{S_j}{K_{S_{X,j}} + S_j} \right) \left(1 - \frac{P - P_{iX,j}}{P_{mX,j} - P_{iX,j}} \right) \left(\frac{K_{iX,j}}{K_{iX,j} + S_j} \right) \quad (1)$$

The total biomass growth based on these two sugars is represented by Equation (2).

$$\frac{dX}{dt} = [\alpha r_{X,1} + (1 - \alpha) r_{X,2}] X \quad (2)$$

The associated glucose and xylose consumption rates are given in Equation (3).

$$\frac{dS_j}{dt} = -\alpha q_{S,\max,j} \left(\frac{S_j}{K_{SS,j} + S_j} \right) \left(1 - \frac{P - P_{iS,j}}{P_{mS,j} - P_{iS,j}} \right) \left(\frac{K_{iS,j}}{K_{iS,j} + S_j} \right) X \quad (3)$$

The rate of ethanol production can be related to the rates of glucose and xylose consumption subject to similar constraints and is given in Equation (4).

$$\frac{dP}{dt} = [\alpha r_{P,1} + (1 - \alpha) r_{P,2}] X \quad (4)$$

with

$$r_{P,j} = q_{P,\max,j} \left(\frac{S_j}{K_{SP,j} + S_j} \right) \left(1 - \frac{P - P_{iP,j}}{P_{mP,j} - P_{iP,j}} \right) \left(\frac{K_{iP,j}}{K_{iP,j} + S_j} \right) \quad (5)$$

The model of Leksawasdi et al. (2001) did not need to account for the production of carbon dioxide

during fermentation. However, in the present investigation, it is necessary to know the amount of carbon dioxide leaving the fermenter when vacuum is used to reduce the concentration of ethanol in the fermenter. We will assume that CO₂ is produced according to stoichiometric equation for the consumption of glucose and xylose. For each kg of glucose or xylose consumed, 0.489 kg CO₂ is produced. It is assumed that the same quantity of CO₂ is produced whether the substrate is used for ethanol production or biomass. It is therefore possible to write the following differential equation to account for the rate of CO₂ produced.

$$\frac{dG}{dt} = -0.489 \left(\frac{dS_1}{dt} + \frac{dS_2}{dt} \right) \quad (6)$$

where dG/dt represents the mass rate of CO₂ production per unit volume of liquid broth.

The 31 parameters of the model can be found in Leksawasdi et al. (2001). With these parameters and the three sets of initial conditions given in the paper, it was possible to reproduce exactly the curves appearing in the publication.

2.2 Simulation Details

To perform the optimization of the process (covered in the next section), the simulation of the complete system must be performed numerous times with different input design parameters. It is not possible to perform the fermentation simulation within UniSim Design such that the simulation of the majority of the system and the optimization algorithm were performed in the VBA environment and UniSim Design was used as a supporting platform for thermodynamic calculations and for simulating the immediate downstream part of the process. The simulation subroutine first obtains from an EXCEL spreadsheet the initial conditions of the fermenter content: X_0 (0.028 kg/m³), S_{10} (150 kg/m³), S_{20} (75 kg/m³), P_0 (0 kg/m³), fermentation time (40 h) and the volume (500 m³). A schematic diagram of the interaction between these computer programs is presented in Figure 2.

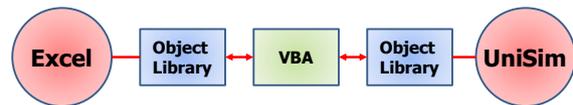


Figure 2: Diagram of simulation communication protocol.

The fermentation is initiated in batch mode such that the system of Equations (1)-(6) is integrated numerically. An additional term in the mass balances for the batch fermentation was added to

account for the entrainment of ethanol and water from the fermenter due to carbon dioxide exiting the fermenter. It is assumed that the carbon dioxide gas stream leaves the fermenter saturated in ethanol and water. When the external flash tank is put in operation, an additional term to the mass balance of each differential equation is added to account for the evaporation rates of ethanol and water.

For each integration step of the mass balance differential equations, the vapour partial pressure of ethanol and water is calculated by passing to UniSim Design the concentration of the fermentation broth and by retrieving the equilibrium mass fraction in the vapour phase (stream 1). With this information, it is possible to perform a complete mass balance for each species within the fermenter and to calculate the mass flow rate and composition of streams 1 and 2 (Figure 1). The information of the combined stream 3 and the desired exit temperature of stream 4 are then sent to UniSim to perform heat and mass balances and to calculate the mass flow rates and concentrations of streams 5, 6 and 7. VBA then retrieves these flow rates and concentrations in addition to the energy required for cooling stream 3 and the power required by the compressor. A screenshot of the two simple systems used in UniSim Design is shown in Figure 3.

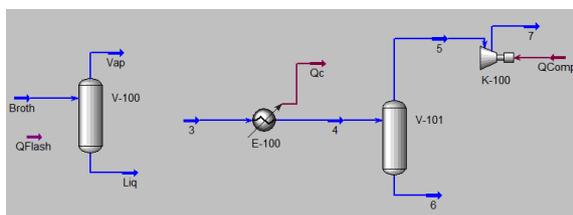


Figure 3: UniSim Design screen capture showing the two processes supporting VBA simulation.

3 OPTIMIZATION ALGORITHM

3.1 Multi-Objective Optimization

The first step to optimize a process is choosing a set of process decision variables that can be manipulated and that have an effect on a series of objective functions. The choice of these decision variables and objective functions need to be performed by experts who have a profound knowledge of the process. In the simple vacuum fermentation illustrative example, three decision variables were first considered (ranges of variation in brackets): (1) the time at which the vacuum system is placed in operation [0, 40 h], (2) the

evaporation rate in the external vacuum flash tank [0, 6 m³/h], and (3) the exit temperature of the condenser (stream 4) [-10, 10°C].

For this optimization study, four objective functions were retained: (1) minimization of overall ethanol lost (kg), i.e. the cumulative amount of ethanol leaving stream 7, (2) maximization of overall ethanol productivity (kg/m³h) based on initial fermenter volume, (3) minimization of residual sugars at the end of fermentation (kg), and (4) minimization of the average consumption by the compressor (MJ/h). This selection is of course not unique and, ideally, the amortized total capital and operating costs per kg of ethanol produced could also need to be considered. However, to investigate the benefits and constraints of using a combination of EXCEL-VBA-UniSim Design, the current example meets this requirement. As mentioned, this simple example must be viewed as a preliminary exploration for the optimization of the complete integrated ethanol plant.

This problem, as summarized in Figure 4, is a multi-objective optimization system. It is desired to determine the values of the decision variables that will maximize the second objective function while minimizing the other three functions. It is possible to combine the four objective functions into a single profit function to be minimized. Even though single objective optimization has been often used in the literature, this method suffers from several disadvantages such as the lack of information about the trade-offs amongst various competing objectives, the difficulty to assign the relative weighting to each individual objective in a single profit function and the convergence on a suboptimal point (local maximum or minimum) instead of global optimum in complex nonlinear problems (Deb, 2001; Haupt and Haupt, 2004).

Even though it requires more computation time, it is significantly more informative to solve the problem as a multi-objective problem with the distinct advantage to generate multiple Pareto-optimal solutions that provide the decision maker or expert a global perspective about trade-offs between conflicting objectives. Other advantages include the ability to optimize functions without requiring information about function derivatives and therefore application in non-convex, non-concave and discontinuous problems (Deb, 2001; Haupt and Haupt, 2004).

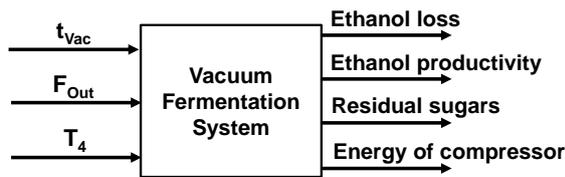


Figure 4: Schematic optimization block flow diagram of the decision variables and objective functions.

3.2 Pareto Domain

The Pareto domain is the set of all feasible solutions that are non-dominated by other solutions in that set. A solution X_1 is said to dominate another solution X_2 if the values of all objectives for X_1 are not worse than those of X_2 , and the value of at least one objective for X_1 is better than the corresponding X_2 (Deb, 2001). Otherwise, both points are non-dominated relative to each other.

Different algorithms exist in the literature to circumscribe the Pareto domain from an initial population of solutions. In this investigation, the dual population evolutionary algorithm (DPEA) was used. This algorithm incorporates the concepts of domination to generate the Pareto domain. The general approach is briefly described as follows (Perrin et al., 1997; Thibault, 2008):

1. An initial set of decision variables is randomly generated within their specified ranges. For each of these points, the values of the objective functions are then calculated as per Section 3.1.
2. The objective functions of all the points are compared to the others (one solution versus another at a time) to determine the number of times a solution is dominated by another.
3. The non-dominated solutions of the population and a portion of the least dominated solutions are used to generate new solutions to replace discarded solutions. To generate a new solution, two kept solutions are chosen randomly and a linear interpolation of their decision variables is performed and the objective functions are calculated.
4. The procedure is repeated until the desired number of non-dominated individuals in the population is obtained.

When the Pareto domain is circumscribed, it can be used per se or the solutions can be ranked according to some preferences expressed by an expert. Two methods are particularly efficient to capture preferences of experts: Net Flow Method and Rough Set Method (Thibault, 2008). In this investigation, only the Pareto domain will be circumscribed and analyzed.

4 RESULTS AND DISCUSSION

4.1 Simulation Statistics

For each function call of the optimizing subroutine, the set of mass balance equations for the fermentation system was integrated over a period of 40 h with a time step of 0.1 h for a total 400 integration steps. Under ideal conditions, it takes approximately 16 to 20 s of computation time to simulate the 40 h fermentation on a Lenovo laptop computer with an Intel 2.49GHz Dual Processor. Sometimes it took much longer to complete a simulation run. The difference in time required undoubtedly depends on the ease to converge to a solution within UniSim even though the flowsheet is relatively simple. The majority of this time is spent communicating with UniSim Design and performing calculation within UniSim. Indeed, to perform a complete function call without resorting to UniSim took less than 1 s.

When the correct communication protocol has been established between VBA and UniSim Design, the simulation of a complete fermentation run was possible and the optimization routine was able to properly approximate the Pareto domain. To obtain a population of 242 non-dominated solutions, it took more than 1500 function calls. A higher number of function calls are required when the number of objective functions is higher. It requires significantly more function calls than a traditional optimization method but it is believed that the payback in having the possibility to examine the trade-offs expressed by the Pareto domain is all worth it.

The use of a metamodel is currently being explored to converge more rapidly to the final Pareto domain. In this method, a neural network model representing the underlying relationship between the decision variables and the objective functions would be developed using the information of the initial population. The metamodel would then be used in the optimization method to determine the Pareto domain. Finally, the Pareto domain obtained using the metamodel would be validated and refined using the more accurate original model. The development of convergence promoter tools is important if one wants to tackle the optimization of the complete ethanol plant in the future. Other techniques are also being evaluated.

4.2 Pareto Domain

A Pareto domain is specific to a set of decision variables and objective functions. Changing some of

the decision variables and/or objective functions will lead to a different Pareto domain. All solutions within the Pareto domain are non-dominated solutions such that in the pairwise comparison of any two solutions, each solution is better for at least one objective function. All feasible solutions outside the Pareto domain are dominated which means that there exists at least one point within the Pareto domain that is better for all four objective criteria.

The main advantage of the Pareto domain is the possibility to clearly observe the compromises that are being made when trying to optimize all four objective functions at the same time. The resulting Pareto domain is a four-dimensional surface containing all potential optimal solutions. Figures 5 and 6 present the four objective functions of the Pareto domain using two-dimensional projections. Each of the 242 points on the graphs represents a different fermentation simulated with a different set of decision variables (start time for vacuum, evaporation rate and condenser temperature).

Figure 5 illustrates very well the compromises that the Pareto domain expresses where an increase in the productivity is accompanied by a greater loss of ethanol. Similar compromise is expressed in Figure 6 where the minimization of residual sugars leads to an increase in the power of compression. Two main reasons explain this compromise: (1) the utilization of a greater quantity of xylose and glucose leads to a higher production of carbon dioxide, and (2) a greater sugar consumption rate requires a higher removal rate of ethanol from the broth in order to reduce product inhibition as shown in Figure 7. Figure 7 shows very clearly that to completely use glucose and xylose by reducing product inhibition, the minimum fermentation removal rate in the flash tank must be nearly 3 m³/h when the flash tank vacuum system is put into operation. Similarly (plots not shown), increasing productivity is accompanied by a decrease in residual sugars and increase in compression energy.

In this investigation, for simplicity and to reduce the number of pieces of equipment, the carbon dioxide stream was combined to the evaporated broth stream. Using a traditional absorption column to capture ethanol would reduce the power of compression at the expense an additional column.

Information about the decision variables are presented in Figures 8 and 9. The histogram of Figure 8 reveals that for the majority of the solutions within the Pareto domain, the vacuum flash tank was put into operation in the vicinity of 20 h, in fact 21.1 ± 5.8 h. This is where the level of ethanol concentration starts to have a greater inhibiting

effect and some of it needs to be removed. It is also more efficient to remove ethanol when the concentration is higher. It would be possible to refine the optimization by adding a stopping time for the vacuum system as another decision or, alternatively, adding the total fermentation time as a decision variable. Either addition would have for benefit to reduce the energy required for compression.

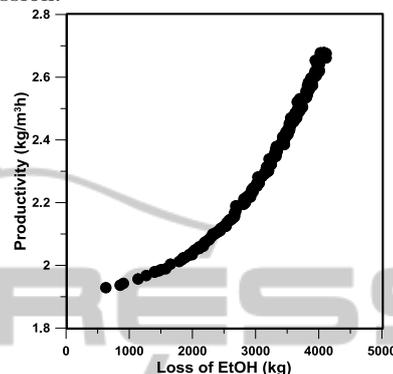


Figure 5: Plot of ethanol productivity versus total ethanol loss during fermentation.

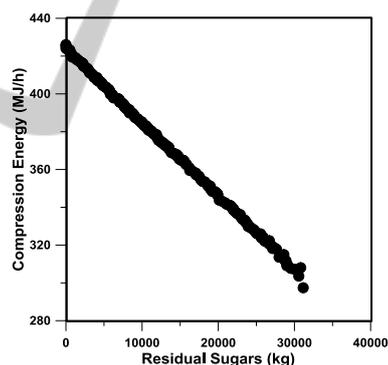


Figure 6: Plot of the energy required for compression versus the residual sugars at the end of fermentation.

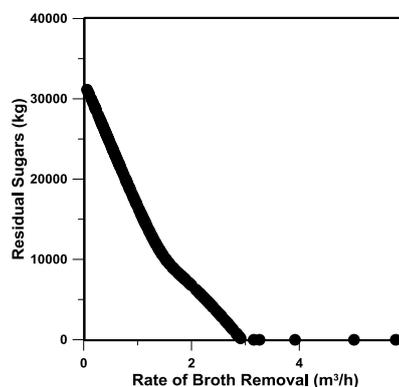


Figure 7: Plot of residual sugars versus rate of broth removal via vacuum boiling.

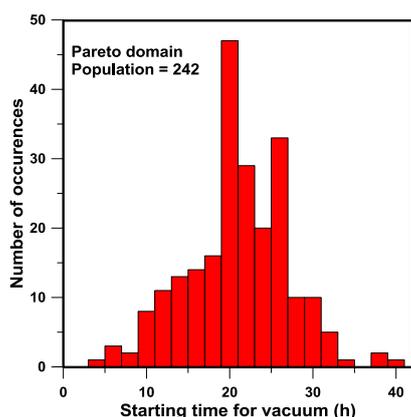


Figure 8: Histogram of the time at which the vacuum flash tank is put into operation for Pareto-optimal solutions.

Figure 9 shows that as the rate of broth removal via the vacuum flash tank is increased, the temperature of the condenser needs to be lowered. For most of the Pareto domain, the condenser temperature hovers in the vicinity of its lower limit of -10°C . Of course, a lower condensing temperature will lead to lower ethanol loss but at greater refrigerant expenses. A lower condensing temperature leads to a higher productivity as shown in Figure 10.

The current fermentation model was developed for a fermenter operating at 30°C such that low vacuum pressure due to thermodynamic limitation had to be used to perform in situ ethanol recovery. If the fermentation could occur at a higher temperature, higher pressure could be used thereby significantly reducing the cost. Microorganisms able to tolerate higher fermentation temperature are currently available but the productivity is yet too low to compete with existing technology (Kumar et al., 2010).

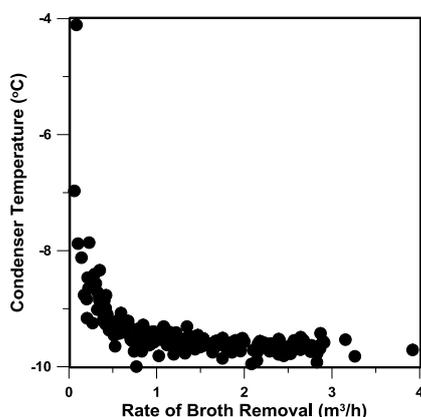


Figure 9: Plot the condenser outlet temperature versus the rate of broth removal.

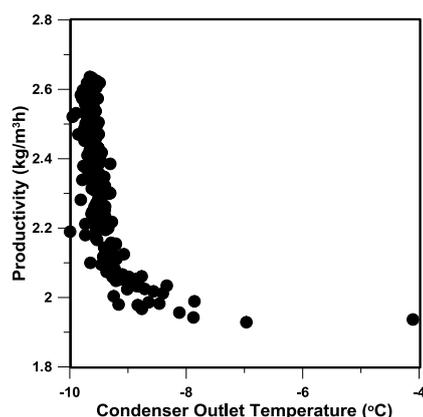


Figure 10: Plot of productivity versus condenser outlet temperature.

5 CONCLUSIONS

The main goal of this paper was to examine, via the simulation and optimization of a simple illustrative example, the ease of combining Excel, VBA and UniSim Design for optimizing industrial plants. This investigation has shown that even for a simple system, the time to access UniSim Design to pass and retrieve information is relatively long. To optimize a more complex plant, the time of simulation will be a limiting factor with the additional risk of not converging to a solution within UniSim Design. It will be necessary to resort to innovative and efficient methods to be able to perform the optimization of a complex plant such as the integrated first and second generation ethanol production plant.

In this investigation, the bulk of the simulation and optimization of the vacuum fermentation system was performed within VBA with UniSim Design performing thermodynamic and downstream processing calculations. The Pareto domain was circumscribed and allowed to observe very clearly the compromises that need to be made when four objective functions, mostly conflicting, were optimized simultaneously.

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