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*Published in:*

32. National Meeting and First International Congress AMIDIQ

*Publication date:*

2011

[Link back to DTU Orbit](#)

*Citation (APA):*

Morales Rodriguez, R., Meyer, A. S., Gernaey, K., & Sin, G. (2011). Technology Evaluation of Process Configurations for Second Generation Bioethanol Production using Dynamic Model-based Simulations. In 32. National Meeting and First International Congress AMIDIQ

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# XXXII National Meeting and First International Congress AMIDIQ

May, 3-6, 2011, Riviera Maya, Mexico

## TECHNOLOGY EVALUATION OF PROCESS CONFIGURATIONS FOR SECOND GENERATION BIOETHANOL PRODUCTION USING DYNAMIC MODEL-BASED SIMULATIONS

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### Abstract

An assessment of a number of different process flowsheets for bioethanol production was performed using dynamic model-based simulations. The evaluation employed diverse operational scenarios such as, fed-batch, continuous and continuous with recycle configurations. Each configuration was evaluated against the following benchmark criteria, yield (kg ethanol/kg dry-biomass), final product concentration and number of unit operations required in the different process configurations. The results has shown the process configuration for simultaneous saccharification and co-fermentation (SSCF) operating in continuous mode with a recycle of the SSCF reactor effluent, results in the best productivity of bioethanol among the proposed process configurations, with a yield of 0.18 kg ethanol /kg dry-biomass.

### INTRODUCTION

Biofuels can potentially contribute to alleviate the current climate change and energy resource challenges, which today's society is facing. Second generation (2G) bioethanol is one of the sustainable biofuels candidates that can potentially address this issue. However, the transfer of these conversion technologies from proof-of concepts to industrial scale has been done on an empirical basis (Aden et al., 2002; Larsen et al., 2008).

Thus, this study has employed the Dynamic Lignocellulosic Bioethanol (DLB1.0) modelling platform (Morales-Rodriguez et al., 2011a), which allowed the quantitative simulation and assessment of diverse process configurations for 2G bioethanol production, thereby providing a basis for evaluation of the most promising process flowsheets. The present work has taken a conventional process configuration as a base case (Margeot et al., 2009), which involves different sections such as, pre-treatment of the substrate, enzymatic hydrolysis of oligosaccharides, co-fermentation of sugars and downstream processes for purification and recovery of most value-added products (see Figure 1), using the dimensions and process conditions proposed by Aden et al. (2002) and Morales-Rodriguez et al. (2011a).

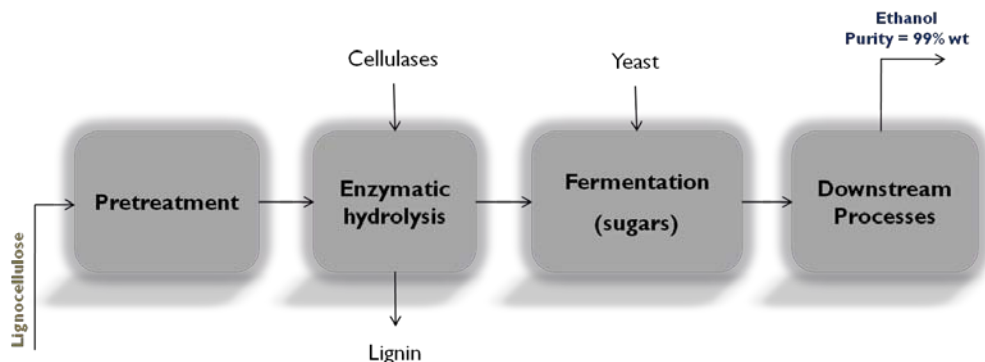


Figure 1 Bioethanol production process from lignocelluloses.

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Each section is represented using dynamic mathematical models. The assessment has been carried out evaluating different process configurations and operational scenarios, such as, fed-batch, continuous and continuous with recycle, mainly found in the enzymatic hydrolysis and co-fermentation sections. Each configuration was evaluated against the following benchmark criteria, yield (kg ethanol/kg dry-biomass), final product concentration and number of unit operations required in the different process configurations. The evaluation has been performed using MatLab/Simulink as a modeling platform.

## MATHEMATICAL MODELS FOR THE DYNAMIC LIGNOCELLULOSIC BIOETHANOL (DLB1.0) MODELLING PLATFORM

The implementation of the model-based simulation framework involved two main parts (Sin et al., 2010): 1) the collection, analysis and identification of the most promising mathematical models for pretreatment (Lavarack et al, 2002), enzymatic hydrolysis (Kadam et al, 2004) and co-fermentation (Krishnan et al., 1999), and, 2) the design, simulation and comparison of different integrated operational scenarios such as, fed-batch, continuous and continuous-recycle. The chosen configurations employ Separate Hydrolysis and Co-Fermentation (SHCF), where - as the name implies - the enzymatic hydrolysis as well as the fermentation of sugars have been performed in different unit operations. In addition, a model for the Simultaneous Saccharification and Co-Fermentation (SSCF) (Morales-Rodriguez et al., 2011b) process was also implemented and its configurations including SSCF reactors were simulated and compared with the results from the base case. Compilation and explanation of the the complete set of used mathematical models can be found in a recent publication (Morales-Rodriguez et al., 2011a).

## PROCESS CONFIGURATIONS FOR 2G BIOETHANOL

Technology evaluation was performed proposing twelve different process configurations employing SHCF and SSCF technologies, nine and three respectively (see Table 1). The distinctions among the process configurations refer to various combinations of fed-batch (FB), continuous (C) and continuous-recycle (C\_REC\_Y) operations.

Table 1. Process configurations proposed for the analysis of the most promising flowsheet.

	Operational Scenario	Acronyms
SHCF	H: Fed-batch –CF: Fed-batch	FB-FB
	H: Fed-batch – CF: Continuous	FB-C
	H: Fed-batch – CF: Continuous-Recycle	FB-C_REC_Y
	H: Continuous – CF: Fed-batch	C-FB
	H: Continuous – CF: Continuous	C-C
	H: Continuous – CF: Continuous-Recycle	C-C_REC_Y
	H: Continuous-Recycle – CF: Fed-batch	C_REC_Y-FB
	H: Continuous-Recycle – CF: Continuous	C_REC_Y-C
	H: Continuous-Recycle – CF: Continuous-Recycle	C_REC_Y-C_REC_Y
SSCF	Fed-batch	SSCF-FB
	Continuous	SSCF-C
	Continuous-recycle	SSCF-C_REC_Y

H: Enzymatic hydrolysis, CF: Co-Fermentation

Process configuration for FB-FB, C-FB, C\_REC\_Y-C\_REC\_Y and SSCF-C\_REC\_Y are illustrated in Figure 2, more details about the rest of the process configurations can be analyzed in material published by Morales-Rodriguez et al. (2011a). For FB-FB process configuration (see Figure 2.a), the feedstock is treated in the pretreatment section (using diluted acid pretreatment), and the product from this operation is passed to the enzymatic hydrolysis unit to perform the conversion of cellulose biomass to glucose. Afterwards, the effluent leaving the enzymatic hydrolysis unit passes through the solid-liquid separator where a percentage of solids is sent to the power generation section (not shown in Figure 2.a), while the liquor stream is sent to the fermentation

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to ferment the glucose into ethanol. The output stream from the fermentation unit is then transferred to the downstream operations to separate the most valuable products (ethanol) and recover those compounds that can be reused in the upstream sections - especially water.

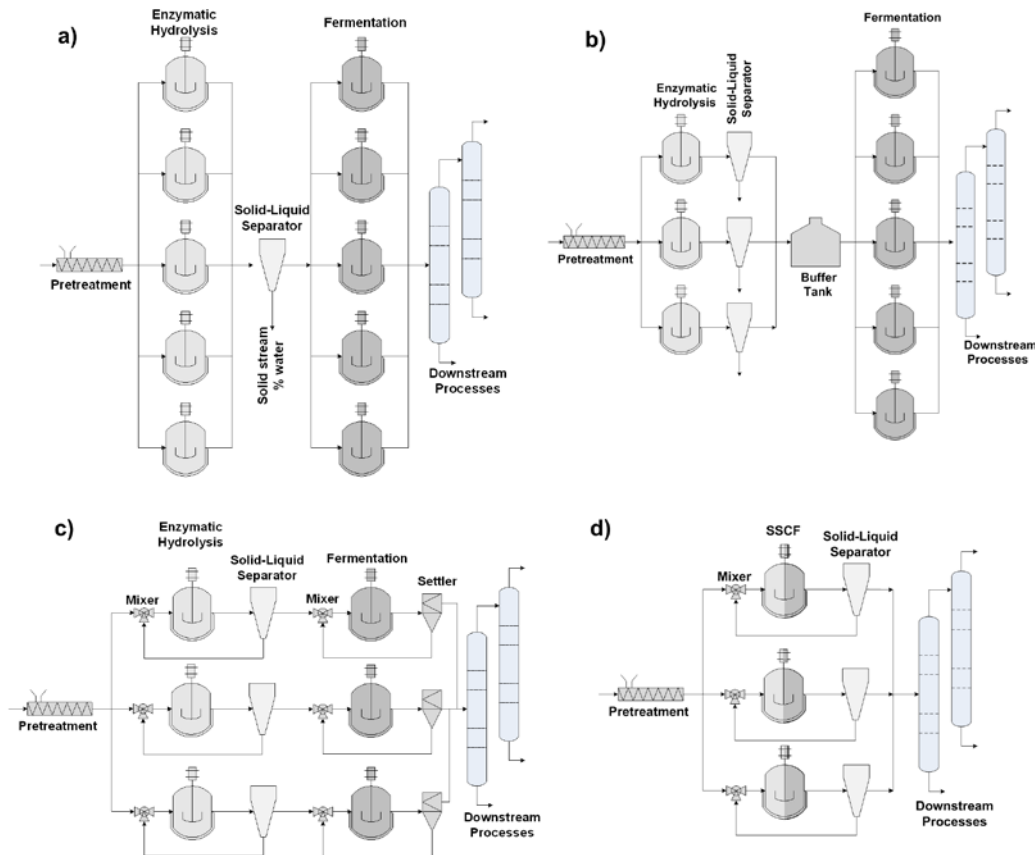


Figure 2 Bioethanol process configurations: a) FB-FB, b) C-FB, c) C\_RECY-C\_RECY, b) SSCF-C\_RECY

With enzymatic hydrolysis in fed-batch mode as a reference, continuous operation requires less unit operations to handle the biomass flow rate from the pretreatment section in order to fulfill the necessary residence time in the hydrolysis reactors (see figure 2.b). Co-fermentation reactors are operated in the same manner as described above. However, some differences are found in other parts of the process flowsheet. For example, in the co-fermentation reactors operating in fed-batch mode (Fig. 1.d), the liquor generated by the solid-liquid separator is fed to the co-fermentation reactors until reaching their maximum capacity while the remaining amount is stored in the buffer tank.

Another process configuration in the enzymatic hydrolysis section is based on the recycle of the insoluble solids stream from the solid-liquid separator (see Figure 2.c). This recycle stream is then mixed with the effluent generated in the pretreatment section before entering the hydrolysis reactor. After solid-liquid separation, liquid stream is conveyed directly to the co-fermentation section where the conversion of sugars into ethanol is accomplished. The settler tank separates the solids from the liquids in the effluent of the fermentor by gravity

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settling and recycles the solids back to the mixer unit which also contains the yeast. This recycling ensures that a high concentration of solids and yeast is maintained in the co-fermentation reactors.

In the SSCF configuration operating in continuous with solid recycle in the output stream (see Figure 2.d), the solid content is mixed with the stream from the pretreatment unit. This action aims to produce the highest possible yield of ethanol per amount of processed raw biomass material, thereby reducing the waste of raw materials in the biofuel production plant.

## OPERATION POLICIES FOR THE PROCESS CONFIGURATIONS FOR 2G BIOETHANOL

When fed-batch processes are used, it is assumed that parallel fed-batch reactors are operated following a batch scheduling scheme consisting of a sequence of different operational phases – for example fill, react, draw, idle – that are repeated over time.

The schedule for fed-batch operation (see Figure 3) describing the operation of the hydrolysis and co-fermentation units (used in the configuration in Figure 2.a) can be understood as follows: for reactor number one a cycle of operation lasts 60 hours. It starts with the loading, an operation that takes 12 hours, and is followed by 36 hours of reaction time. Finally it ends with 12 hours of drawing/emptying the reactor contents. Upon the completion of the first cycle, the next cycle starts again by repeating the same schedule. The first fermentation reactor therefore starts after 48 hours then following the 12, 36 and 12 hours scheduling (Figure 3).

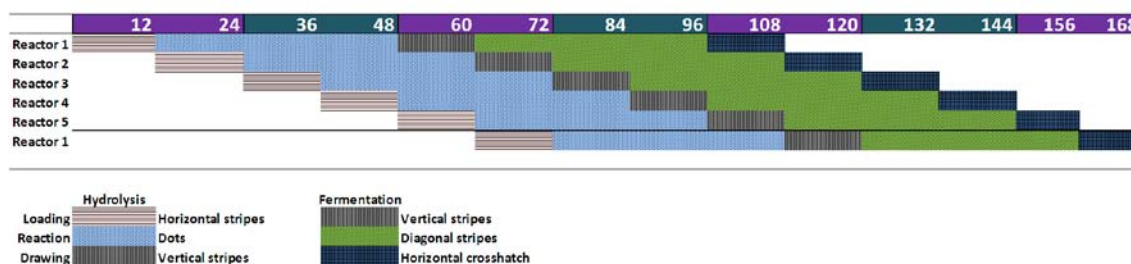


Figure 3 Scheduling for FB operation in the hydrolysis and fermentation sections.

Regarding the co-fermentation unit, the loading period is assumed to start simultaneously with the drawing of the contents from the hydrolysis unit, thus assuming that an ideal solid-liquid separation operating in steady state is present between hydrolysis and co-fermentation. It is important to remark that a buffer tank is needed after the hydrolysis units (operating in continuous) to buffer the continuous flow before it is fed to the fed-batch operated fermentors (see figure 2.b).

## BENCHMARK CRITERIA FOR COMPARISON OF THE DLB1.0 SIMULATION OF THE CONFIGURATIONS

The comparison of the performance of the different process flowsheets has been performed by using as evaluation criteria: the ethanol/dry-biomass ratio, the fraction of unreacted raw material and the final ethanol concentration.

The ethanol/dry-biomass ratio has been calculated on the basis of the total amount of ethanol that is transferred to the downstream processing section as follows:

$$R_{Et/dry-biomass} = \frac{Total\ Mass\_Et}{Total\ Mass\ Dry\_Biomass} \quad (1)$$

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The fraction of unreacted raw material (URM) has been calculated using the accumulated dry-biomass (ADB) in the process plus the dry-biomass separated in the solid-liquid separator unit versus the total amount of dry-biomass fed in the operating time (Equation 2):

$$URM = \frac{ADB + \text{Solid stream from } S-L \text{ separator}}{\text{Total Mass Dry\_Biomass}} \quad (2)$$

## RESULTS: TECHNOLOGICAL EVALUATION

Among the different DLB1.0 simulations of the configurations, the maximum ethanol yield obtained is found for the SSCF process configuration operated with continuous feed with recycling of the solids (see Figure 2.d). This outcome can be explained to a large extent by the positive effect of the recycle, which improves the process efficiency in two ways: (i) by recycling the unused raw material (that is cellulose) the amount of raw material wastage is decreased – this is illustrated in Figure 4.b where the amount of unreacted raw material for the SSCF\_C\_RECYC is 0, (ii) by recycling the yeast the concentration of microorganisms maintained in the reactor is increased significantly to 9.75 % (w/v) in comparison to 2.13% (w/v) in the SSCF-C configuration.

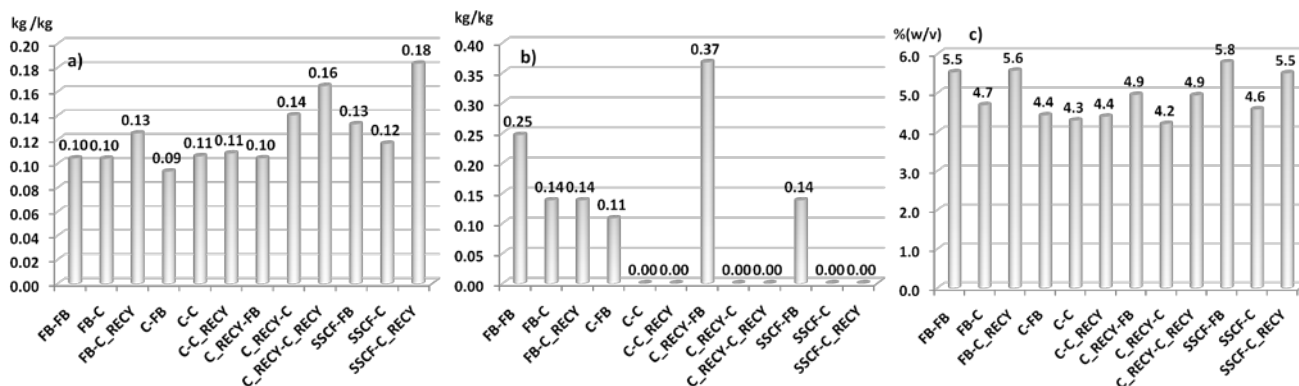


Figure 4 Simulation results for the proposed configurations: a) Ethanol/dry-biomass ratio, b) unreacted raw material fraction, and c) ethanol concentration.

The second best yield was found for a SHCF type process where both the hydrolysis and the co-fermentation units are operated continuously with recycle (C\_RECY-C\_RECY) (Figure 2.c). This result demonstrates also that continuous operation with a recycle has the major positive impact among the process flowsheet configurations.

The third best yield was found for a SHCF type process configuration where hydrolysis is operated continuously with recycle while the co-fermentation is just in continuous mode (C\_RECY-C). The 0.0245 kg ethanol/kg dry-biomass decrease in the ethanol yield is attributable to the lack of recycle in the co-fermentation reactor. Compared to the scenario with the best performance, there is 5.5 % of the glucose and 71.2% of the xylose unfermented (with respect to the feed) in the effluent of the fermentor.

The SSCF fed-batch (SSCF-FB) operation is ranked fourth, even though a certain fraction of unreacted raw material is presented (0.13) (see Figure 4). This configuration presents the highest ethanol concentration (5.8 % w/v) in the final amount of product. Fed-batch operation for the conversion of cellulose to glucose and continuous operations with a recycle stream in the co-fermentation of glucose and xylose to ethanol (FB-C\_RECY), is the option ranking 5<sup>th</sup> among the tested configurations.

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The remaining process flowsheet configurations were found to perform poorly with yields below 0.11 kg ethanol/kg dry biomass.

## CONCLUDING REMARKS

A number of scenarios have been proposed, analyzed and compared for finding the most feasible process technology for integrated operation of various lignocellulosic bioethanol process configurations using a dynamic modeling framework. The results showed that four of those configurations produced the highest ethanol yields per amount of dry-biomass: SSCF-C\_REC\_Y, C\_REC\_Y- C\_REC\_Y, C\_REC\_Y-C and SSCF-FB (0.18, 0.16, 0.14 and 0.13 kg/kg, respectively).

Further analysis on these process configurations has been performed by Morales-Rodriguez et al., (2011a). A sensitivity analysis of the reaction volume with respect to process yield for ethanol, has shown the possibility of reducing the number of equipments for various process configuration, without compromising the bioethanol production yield. The advantages of technology evaluation based on the DLB1.0 simulations can be seen from three different perspectives: a) maximize the yield of the raw material, b) the optimized operation point of view: get more out of the existing plant capacity/equipment, c) the process design point of view: use a minimum capacity/equipment to achieve better process performance (design target), which has a direct impact on the capital cost of the bioethanol plant.

## ACKNOWLEDGEMENTS

The authors acknowledge the Mexican National Council for Science and Technology (CONACyT, project #145066) for the financial support on the development of this project.

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