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Resource Efficiency Studies using a New Operator Training Simulator for a Bioethanol Plant

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Biofuel production plants are expected to significantly contribute to an environmentally sustainable future. However, a prerequisite for this goal is the resource conserving and energy efficient operation of these plants. Complex process dynamics are supposed to have an important influence on resource and energy efficiency of biofuel plants. This leads to strong demands on plant operators and automation systems. In this contribution a newly developed operator training simulator (OTS) is used to demonstrate the influence of process control and automation strategies on the sustainable operation of a bioethanol plant. The OTS presented here is based on mechanistic and dynamic process models describing the unit operations and some additional equipment such as valves, pumps, etc.. The models were verified using pilot plant data and have been implemented in the control system and simulation software WinErs. Automation sequences for the full plant have been developed using GRAFCET. Simulation experiments with the operator training simulator of the bioethanol production plant clearly indicate the strong influence of operational strategies and conditions on the resource efficiency and bioethanol yield of the process. The operational strategies and conditions for the bioethanol fermentation unit, the cross flow unit as well as the rectification unit and the overall process may lead to a variation of the energy demands for ethanol production of 48 %.

1. Introduction

Considerable research has been carried out to enhance the sustainability of bioethanol plants by improving their plant design and extending the spectrum of utilizable raw materials (Walker, 2011). However, bioethanol plants consist of highly interacting unit operations such as bioreactors, membrane filtration units, distillation columns etc. with complex dynamic behaviour. Thus, operational and control strategies are supposed to have a strong influence on the resource efficiency of these plants. Despite this relevance, no systematic investigations regarding the impact of plant operation and control on the resource efficiency of bioethanol plants have been published in the scientific literature (Kuntzsch, 2014). One reason for the lack may be the high experimental effort, which would be required to perform such investigations on real complex plants.

Although modern plant simulators, such as Aspen Plus or ChemCad, provide tools for dynamic plant simulations as used by Li (2010) or Claus (2009), they do not provide powerful tools to model control loops and automation systems of bioethanol plants. Operator training simulators for the process industry typically combine dynamic process models with models of the automation and control system (Klatt, 2009). However, no simulator or simulation study has been published so far, investigating the influence of operational and control strategies on the resource efficiency of bioethanol plants.

Here we present a newly developed operator training simulator for a small pilot scale bioethanol production plant, including the start up and shut down procedures, similar to a full plant. Using this new complex simulator we will demonstrate that carefully designed control strategies may significantly enhance the resource efficiency of bioethanol production processes.

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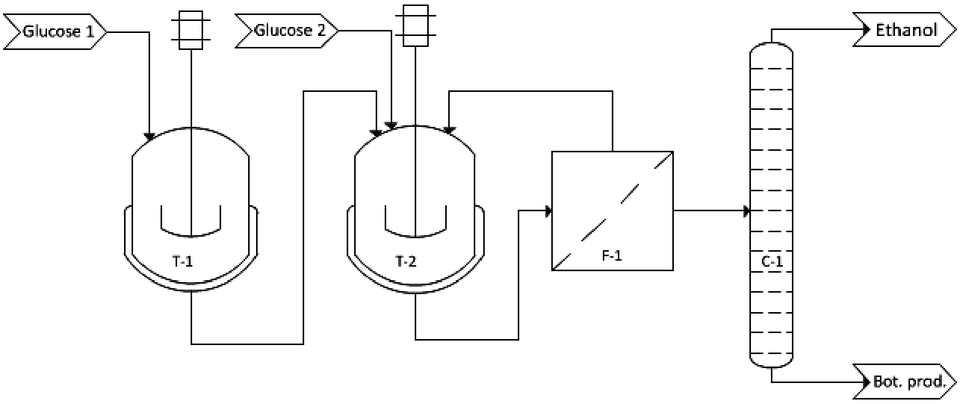


Figure 1: Bioethanol plant with bioreactor T-1, bioreactor T-2, cross-flow unit F-1 and rectification unit C-1

2. Bioethanol plant

The process, which is used for the investigation in this work, is composed of two bioreactors, a cross-flow filtration unit and a rectification column (Figure 1). In this process the yeast *Saccharomyces cerevisiae* is used as the ethanol producing organism. In bioreactor T-1 the starter culture is produced aerobically and then transferred to T-2. Bioreactor T-2 is operated anaerobically to efficiently convert the carbon source to ethanol. The maximum working volume of the bioreactors is 15 L. The ethanol-yeast-water suspension is fed to a cross-flow unit to retain the biomass and recycle it to the bioreactor T-2. This enables throughputs in bioreactor T-2 beyond washout of the yeast cells and thus increases the productivity of the plant. The clarified ethanol-water solution is finally fed to a normal pressure rectification unit, were the top product mainly contains ethanol and the bottom product mainly contains water plus residual substrates and side products with low vapour pressure. The bottom product may be fed to a biogas plant (Blesgen and Hass, 2010). The bioethanol plant may be operated in batch, fed-batch and continuous mode. A more detailed description can be found in Kuntzsch (2014).

3. Bioethanol plant simulator

The simulator shall be used to investigate the impact of process control strategies in the bioethanol plant on its resource efficiency. Thus, the simulator must be capable of describing the dynamic behaviour of the full plant, including the (bio-)reaction kinetics, the kinetics of heat and mass transfer, the dynamics of the bioreactors, cross-flow filtration unit or the rectification column as well as the dynamic behaviour of the valves, pumps, compressors, heat exchangers, measurement devices and other plant elements. Furthermore, a model of the automation system of the process is required, as the plant automation may significantly influence the overall process dynamics.

A shell structure has been shown to be very effective to structure the simulator models (Blesgen and Hass, 2010). This structure was adapted to the bioethanol plant. The inner shell comprises the kinetics sub-models. These are embedded in the unit operation sub-model, describing the type of reactor or unit operation. Around the unit sub-model the plant sub-model is built, combining the individual unit operations to a full plant (Figure 2, left).

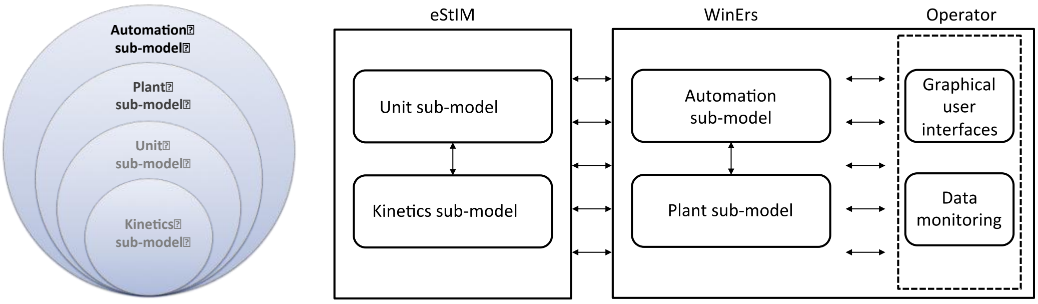
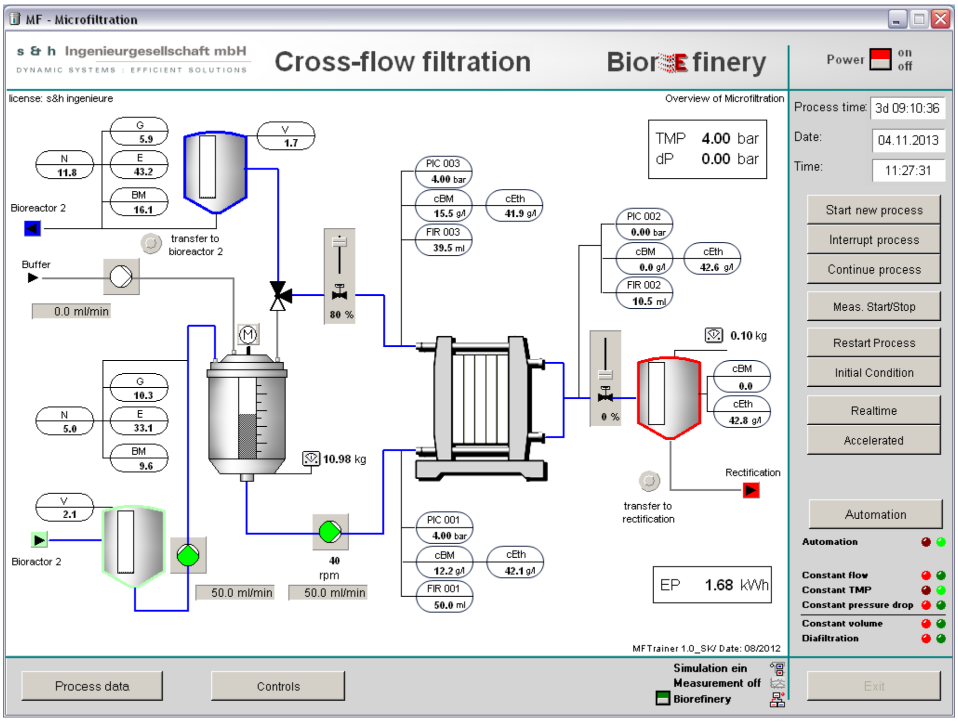


Figure 2: Structure of the bioethanol plant simulator. Left: Shell structure of the simulator, adapted from Blesgen and Hass (2010). Right: Connection of eStiM-models and WinErs (Kuntzsch, 2014)



Process time: 3d 09:10:36
Date: 04.11.2013
Time: 11:27:31
TMP 4.00 bar
dP 0.00 bar
EP 1.68 kWh
G 5.9
E 43.2
BM 16.1
N 11.8
V 1.7
0.0 ml/min
G 10.3
E 33.1
BM 9.6
N 5.0
V 2.1
50.0 ml/min
50.0 ml/min
40 rpm
80 %
10.98 kg
PIC 003 4.00 bar
cBM 15.5 g/l
cEth 41.9 g/l
FIR 003 39.5 ml
PIC 001 4.00 bar
cBM 12.2 g/l
cEth 42.1 g/l
FIR 001 50.0 ml
PIC 002 0.00 bar
cBM 0.0 g/l
cEth 42.6 g/l
FIR 002 10.5 ml
0.10 kg
0 %
cBM 0.0
cEth 42.8 g/l
Automation
Constant flow
Constant TMP
Constant pressure drop
Constant volume
Diafiltration
Simulation ein
Measurement off

Figure 3: Graphical user interface of the cross-flow filtration unit

The individual mathematical models are formulated as systems of non-linear differential equations. The kinetics and unit sub-models have been implemented using the software package eStIM, developed at the Hochschule Bremen (Kuntzsch, 2014). The plant and automation sub-models were directly implemented in WinErs, a process control and simulation software (Schoop, 2012). Both software systems are using the Runge-Kutta-Algorithm of 4th order to compute systems of differential equations. This algorithm is precise and can be utilized in real time systems. The models implemented in eStIM were embedded into the process control system using a DLL interface block, provided by WinErs. WinErs was also used to develop the graphical user interface/operator screens and perform the data monitoring. The individual units were linked by appropriate interfaces (Figure 2, right).

The bioethanol plant simulator consists of four individual unit operation simulators: bioreactor 1, bioreactor 2, cross-flow filtration and a rectification column. All operator screens have a common general structure in order to facilitate easy operation of the individual unit operations as well as the full plant (Figure 3). More detailed descriptions of the bioreactor simulator and the rectification column simulator models may be found in Hass, Kuntzsch et al. (2012) or in Kuntzsch (2014). In the subsequent section the cross-flow filtration model will be presented briefly. Additionally, a sensor model will be shown as example for a supplementary device model.

3.1 Cross-flow filtration

The feed to the membrane module $\dot{V}_F$ contains yeast cells, glucose, other substrates, ethanol and water (Figure 4). Outputs are the cell free permeate $\dot{V}_{perm}$ and the retentate $\dot{V}_{ret}$ with an enriched biomass concentration. The liquid phase concentrations of the solutes (ethanol, glucose) remain unchanged by this unit operation. The permeate flux $\dot{V}_{perm}$ through the membrane mainly depends on the operating variables trans membrane pressure (Δp_{TMP}) and feed flow rate $\dot{V}_F$:

$$\dot{V}_{perm} = \frac{\Delta p_{TMP}}{\eta_F(R_M + r_C h_C)} \qquad (1)$$

η_F is the fluid viscosity. R_M and r_C are the membrane resistance and the specific filter cake resistance, respectively. The filter cake height h_C is a function of the feed flow rate. High flow velocities reduce h_c, as the cells forming the filter cake are carried away due to frictional forces.

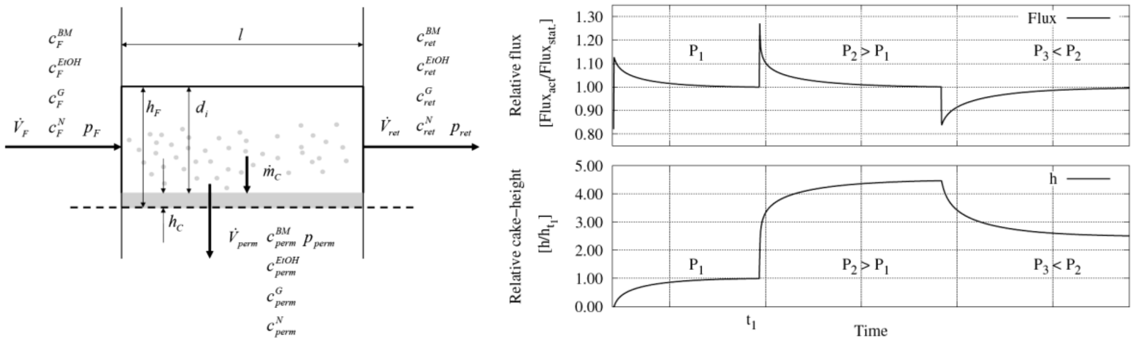


Figure 4: Left: Structure of the cross-flow filtration model. Right: Relative cake height and relative flux as functions of the time at different pressures, where $p_1 < p_3 < p_2$

Increasing trans membrane pressure and a decreasing filter cake height result in an increasing permeate flux, which in turn leads to an increasing filter cake build up. The larger the permeate flux and the higher the biomass concentration in the feed, the more rapid the filter cake build up.

The dynamics in the cross-flow filtration unit results from the filter cake build up and the change in the biomass concentration in the feed, which in turn is a result of cell growth in the bioreactor and the biomass recycle from the cross-flow filtration unit. A secondary effect is the dilution in the storage tanks connecting the unit operations. The right side of figure 4 illustrates the permeate flux as a function of time at trans membrane pressures $p_1 < p_3 < p_2$ as modelled with the cross-flow simulator and previously described by Rautenbach (1997). It may be seen from figure 4, that as the filter cake is build up with time the flux decreases and vice versa. The higher the trans membrane pressures the higher the filter cake. However, the permeate flux almost remains constant. Higher trans membrane pressures compensate for the increasing height of the filter cake.

3.2 Sensor model

Some sensors in the plant, such as pH and pO_2 probes, offgas analytics or temperature sensors do show a time delay, until they show the “real” value of a state variable. This may have a significant impact on the control loop behaviour. Thus, the dynamics of the sensors has been modelled by differential equations of first order, which are called PT_1-systems in control engineering:

$$T_1 \cdot \dot{x}(t) + x(t) = G \cdot y(t) \tag{2}$$

In Eq(2) T_1 denotes a time constant, $x(t)$ is the output signal of the measurement device, $y(t)$ is the actual value of the state variable as calculated by the unit operation model and G is the system gain. Figure 5 shows the step response of this system, when Gaussian noise is applied to the measurement values $x(t)$.

3.3 Automation model

Here, the plant automation system was modelled on two levels. First, the required PID-control loops were implemented as in the real plant as well. Second, the operational sequence for plant operation was modelled using GRAFCET (**G**raphe **F**unctionnel de **C**ommande **E**tapes / **T**ransitions, IEC 60848, IEC 1131-3), which is a sequential function chart. A GRAFCET-plan consists of steps, transition conditions and actions, which are connected by functional lines (Gerneay et al, 2000). Any operational sequence for a process can be described graphically using GRAFCET (Figure 5).

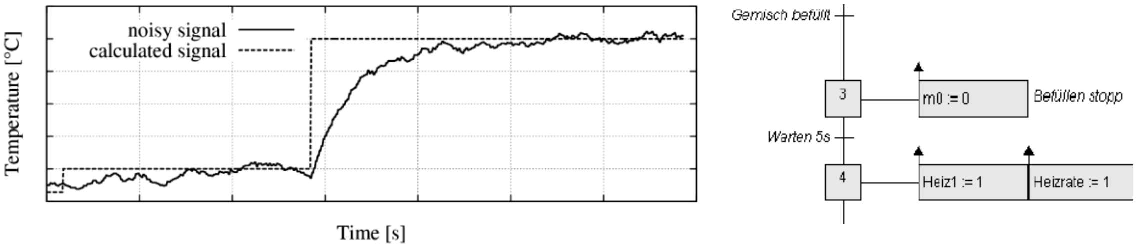


Figure 5: Left: Step response function of a temperature sensor. Right: Part of a GRAFCET-plan

The process control system WinErs provides an inbuilt GRAFCET editor, which also allows to compile the plan, producing an executable sequence control scheme.

In this work, GRAFCET-plans were used, to realize different operational sequences with the simulator. In this way different operational sequences could be compared. Performance differences due to process handling by operators were avoided.

4. Simulation studies and discussion

The bioethanol plant simulator was used to perform two simulation studies. First, the impact of different operational strategies on the resource efficiency in a single bioreactor with aerobic yeast growth and anaerobic ethanol production was investigated. Second, a complex plant operation was investigated, when running the process in a semi-continuous mode with different substrate concentrations in the feed.

4.1 Case 1: bioreactor operation

If only one bioreactor is used for ethanol production, the duration of the aerobic growth phase and the duration of the anaerobic ethanol production phase do have an impact on the consumption of substrates as well as on the amount of ethanol produced in a given time.

In order to obtain a reasonable biomass yield with respect to the carbon source during the aerobic growth phase, substrate was fed in an exponential manner according to the exponential growth and substrate consumption. Glucose concentrations below 3 kg m^{-3} were maintained in the bioreactor in this phase. After 6, 8, 10 or 12 hours operating time the process was switched from aerobic growth to anaerobic ethanol production. The processes with 10 and 12 hours of aerobic growth were finished after 19 and 17 hours, when the maximum achievable ethanol concentration was reached. The other processes were finished after 24 hours. As can be seen from table 1 the process appears to have an optimum ethanol yield from glucose, if the aerobic growth phase ends after 8 hours. However, a longer growth phase does lead to higher ethanol amounts and shorter process times.

4.2 Case 2: semi-continuous whole plant operation

In the second simulation study a full plant was operated. The simulation started with aerobic growth of yeasts in bioreactor 2 in a fed-batch mode to maintain moderate glucose concentrations below 3 kg m^{-3}. In scenario A a glucose concentration of 500 kg m^{-3} in the feed was used. In scenario B the glucose concentration was 250 kg m^{-3}. After 12 h operation time the anaerobic phase began. The continuous operation of the bioreactor started, when a volume of 10 L was reached in the vessel. Surplus media was transferred to the cross-flow filtration, where the suspended biomass was separated from the culture broth and recycled to the bioreactor. The cell free ethanol-water mixture was transferred to a buffer tank. In scenario A 14.3 L of a water-ethanol solution were produced (ethanol concentration: 120.7 kg m^{-3}) within 27 h. In scenario B 28.4 L of water-ethanol solution were produced (ethanol conc: 68.1 kg m^{-3}) within 24 h. The buffer tank solutions then were partially transferred to the rectification column for start-up of the column. After reaching an equilibrium state, the continuous operation of the column was initiated. Finally, in scenario A 2.3 L of 91 vol% ethanol solution were produced, in scenario B 2.6 L of the 91 vol% ethanol solution could be obtained. Table 2 shows important process performance indicators.

In scenario A the total glucose and N-source consumption were higher as compared to scenario B, although less ethanol solution could be produced in scenario A. Although the cultivation process of scenario B appears to be slightly advantageous as compared to scenario A, the total energy demand for scenario A is only 52% of the energy demand for scenario B. The ethanol specific energy demand of scenario A is 41% less than the specific energy demand of scenario B. Thus, the operational conditions may have a considerable impact on the resource efficiency of the bioethanol process.

Table 1: Ethanol production and resource consumption

Aerobic phase length (h)	EtOH produced (kg)	EtOH per glucose (kg kg^{-1})	EtOH per N-source (kg kg^{-1})
6	0.80	0.55	6.9
8	1.90	0.60	5.1
10	2.30	0.55	3.0
12	2.60	0.47	2.0

Table 2: Comparison of scenarios A and B

	Scenario A	Scenario B
Cultivation		
Glucose	5.176 kg	4.447 kg
N-source	1.281 kg	1.166 kg
Energy	0.41 kWh	0.44 kWh
Cross-flow filtration		
Energy (Pump)	0.37 kWh	0.77 kWh
Rectification		
Energy	7.56 kWh	14.70 kWh
Ethanol (91 vol-%)	2.3 L	2.6 L
Total energy	8.34 kWh	15.91 kWh

5. Conclusions

A new type of process simulator for bioethanol production plants was developed during the presented work. The general framework of the operator training simulator enabled the combination of individual unit operation simulators to a full plant simulator. This new type of simulator was used for the investigation of the influence of operational strategies on the resource efficiency of individual unit operations as well as of complete plants. It could be shown, that the selection of the most effective operational strategy and operating conditions in the bioethanol plant under consideration may reduce its energy demand by 48 %.

In future work the simulator will be used for the systematic development of operational strategies and subsequently for the efficient training of plant operators with respect to their influence on a sustainable plant operation. Due to its modular structure the simulator may be adapted to other plant sizes or configurations with reasonable effort and thus provides a very efficient new means to improve resource and energy efficiency of biofuel plants during their actual operation.

Research on new biorefinery concepts will be of increasing importance in the future. In parallel to this research corresponding training simulators will be developed using the methods and tools presented in this paper. The simulators then contribute to an accelerated start-up of the new processes and further enhance their resource efficiency by well-designed operational strategies.

Acknowledgement

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