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COMPARING A DYNAMIC FED-BATCH AND A CONTINUOUS STEADY-STATE SIMULATION OF ETHANOL FERMENTATION IN A DISTILLERY TO A STOICHIOMETRIC CONVERSION SIMULATION

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Abstract – An autonomous sugarcane bioethanol plant was simulated in EMSO software, an equation oriented process simulator. Three types of fermentation units were simulated: a six parallel fed-batch reactor system, a set of four CSTR in steady state and one consisting of a single stoichiometric reactor. Stoichiometric models are less accurate than kinetic-based fermentation models used for fed-batch and continuous fermenter simulations, since they do not account for inhibition effects and depend on a known conversion rate of reactant to be specified instead. On the other hand, stoichiometric models are faster and simpler to converge. In this study it was found that the conversion rates of sugar for the fermentation systems analyzed were predictable from information on the composition of the juice stream.Those rates were used in the stoichiometric model, which accurately reproduced the results from both the fed-batch and the continuous fermenter system.

Keywords: Bioethanol; Fed-batch fermentation; Continuous fermentation; Stoichiometric fermentation; Simulation.

INTRODUCTION

Ethanol is a mandatory additive to gasoline in several countries and states in the USA, as well as a widely used vehicular biofuel in Brazil since 1975. Its reliance on food crops such as sugarcane and corn, however, has aroused much criticism both from the academy (Rathman et al., 2010; Tilman et al., 2009) and the general public (Runge and Senauer, 2007). Second generation bioethanol, obtained from lignocellulosic materials, has raised interest from the scientific community as a more sustainable alternative (Naik et al., 2010). The challenge of designing a viable second generation biorefinery has led to much research in which industrial facilities with integrated first and second generation processes were simulated (Dias et al., 2012a, 2012b; Furlan et al., 2012, 2013; Ojeda et al., 2011; Palacios-Bereche et al., 2013).

Bioethanol is produced in bioreactors in which reducing sugars obtained from sugar crops, starch crops or hydrolyzed lignocellulosic biomass are fermented, mostly by yeasts of the species *Saccharomyces cerevisiae* (Lin and Tanaka, 2006). These yeasts are used due to their high resistance to relatively harsh environmental conditions such as low pH (4.5 to 5.0) and high ethanol concentrations

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(10% to 12% volume/volume), which are extreme for most microorganisms, including undesirable competitors that could decrease the product yield of the fermentation (Gao and Fleet, 1988). Despite the relatively high tolerance to ethanol, this product of fermentation is toxic to yeasts themselves and inhibits the reaction kinetics.

Most computer simulations of ethanol distilleries use stoichiometric conversion models to represent fermentation reactors. There are advantages in using such models instead of those involving reaction kinetics, such as fast convergence and simplicity of modeling and optimization, since dynamic fed-batch models require specialized optimization algorithms (Roubos et al., 1999). However, stoichiometric models typically do not incorporate the aforementioned inhibition effects that could hinder the product output of the reaction. Instead, they rely on previously known information on the conversion rate of substrate.

Many reaction rate laws have been proposed to model the fermentation reaction considering inhibition effects (Ghose and Tyagi, 1979; Han and Levenspiel, 1988; Lee et al., 1983; Levenspiel, 1980). The model of Ghose and Tyagi (1979) is one of the most commonly employed, accounting for product and substrate inhibition effects. It is an unstructured and non-segregated model, meaning that the cell culture is seen as a single component uniformly distributed throughout the solution (Dutta, 2008).

Fermentation reactor models that make use of kinetic models are seldom used for plant-wide simulations, especially to represent fed-batch reactor systems. This work investigates to which extent a stoichiometric model is trustworthy to represent high yield fermentations in which inhibition effects are relevant to the reaction kinetics.

METHODOLOGY

EMSO (Environment for Modeling, Simulation, and Optimization) is a tool for modeling, simulation and optimization of dynamic systems using an equation-oriented approach (Soares and Secchi, 2003). This software offers a free and open-source model library and it allows users to create their own models. Its modeling language follows an object-oriented paradigm, which enables inheritance and composition. Such features allow the creation of complex models through the extension and combination of simpler ones (Rodrigues et al., 2010). Another important characteristic of this software is its extensibility through plug-ins, which enhance its flexibility.

Three models of fermentation systems were created, namely, a traditional stoichiometric reactor, dynamic fed-batch reactors (Fig. 1) and continuous tank reactors in steady state (Fig. 2). The two latter assume perfect mixture condition, isothermal operation, constant density for all liquid streams and follow the reaction kinetic law of Ghose and Tyagi (1979).

The mass balances employed in the fed-batch and continuous fermenter models, as well as the Ghose-Tyagi kinetic equations are shown in Equations 1 through 6. The values of the fermentation parameters in those equations are those established by Ghose and Tyagi (1979) in their original work and are shown in Table 1. Sensitivity tests were done for the kinetic parameters to assess the robustness of the model. In fed-batch reactors the inlet volumetric flow rate ($F^{in}(t)$) and outlet flow rate ($F^{out}(t)$) are

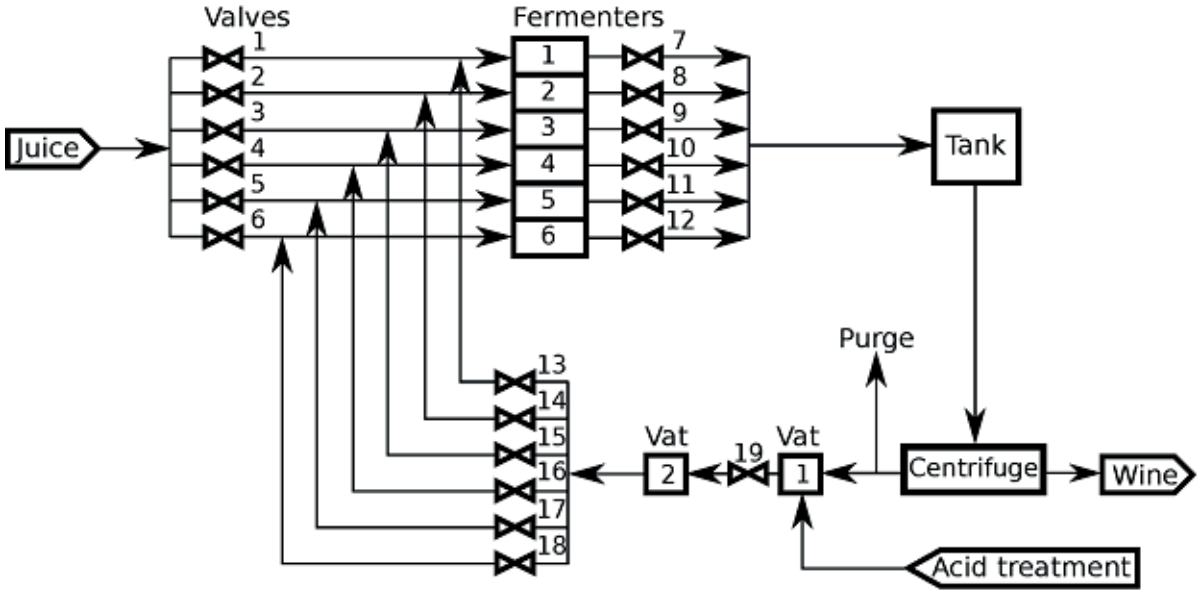

Figure 1. Block diagram for the fed-batch fermenter system with six parallel reactors and cell recycle.

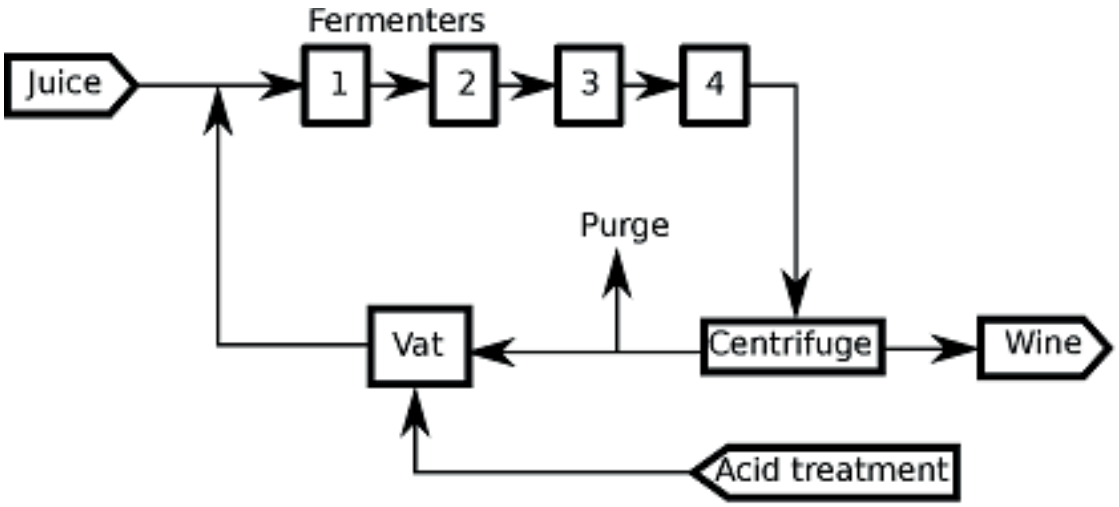

Figure 2. Block diagram for the continuous fermenter system with four reactors and cell recycle.

Table 1. Fermentation parameters employed in the simulations.

Parameter	Value
$\mu_{max}(h^{-1})$	0.36
$k_d(h^{-1})$	0.0083
$k_s(kg/m^3)$	0.48
$k_i(kg/m^3)$	203.5
$C_P^*(kg/m^3)$	90.0
$Y_{X/S}(kg_{cell}/kg_{substrate})$	0.035
$Y_{P/S}(kg_{product}/kg_{substrate})$	0.48

determined by the valves next to each fermenter and their behaviors are approximations to a rectangular function (Carver, 1978). In the continuous fermenter, the inlet and outlet volumetric flow rates are constant and equal.

Total mass balance:

$$\rho \frac{dV}{dt} = \rho \cdot (F^{in}(t) - F^{out}(t)) \quad (1)$$

Component mass balance:

$$\frac{dC_i}{dt} = \frac{F^{in}}{V} \cdot (C_i^{in} - C_i) + r_i \quad (2)$$

Reaction rate of sugars:

$$r_S = -\mu \cdot C_X \frac{1}{Y_{X/S}} \quad (3)$$

Reaction rate of cell biomass:

$$r_X = (\mu - k_D) \cdot C_X \quad (4)$$

Reaction rate of ethanol:

$$r_P = \mu \cdot C_X \frac{Y_{P/S}}{Y_{X/S}} \quad (5)$$

Kinetic model of Ghose-Tyagi:

$$\mu = \frac{\mu_{max} \cdot C_S}{k_S + C_S + \frac{C_S^2}{k_I}} \cdot \left(1 - \frac{C_P}{C_P^*}\right) \quad (6)$$

Fed-batch reactors were designed in accordance to the specifications of an industrial mill from São Paulo state,

Brazil. Each reactor works with a complete fermentation cycle of 12h, comprising half an hour for the inoculation of yeast cream (with composition of 30% biomass on a wet basis), five hours for juice feeding, three hours of batch, one hour and a half for discharging and two hours of cleaning in place and inactivity until the next cycle. Six fed-batch fermenters were instantiated and the fermentation cycle of each one is offset by two hours in relation to the next. The volume profile of one single reactor (Fermenter 1) during a full cycle as well as the behavior of each reactor at each time is illustrated in Fig. 3.

Contrary to the fed-batch, both the continuous fermentation reactors and the stoichiometric reactor were modeled to run in steady state. Continuous fermentation was modeled with four reactors arranged in series. Their total volume is equal to the average working volume of the fed-batch fermentation system and the volumes of each fermenter were determined by a particle-swarm optimization (PSO) algorithm with the goal of maximizing the total production of ethanol in the centrifuged wine.

For the stoichiometric reactor, one single block was used to represent the whole fermentation process. The conversion equations are expressed by Equations 7 to 9, which neglect the participation of water, carbon dioxide and other substances involved in the conversion of glucose to biomass. The cell and product yield coefficients ($Y_{X/S}$ and $Y_{P/S}$) are the same as those used in fed-batch and continuous fermentation. The conversion of sugar (X) for different inputs is not immediately known, since the stoichiometric model cannot predict the effects of inhibitions, hence it was calculated in the kinetic fermentations and applied to the stoichiometric models.An attempt was made to find a general trend in the conversion in order to improve the stoichiometric model using an equation to estimate the conversion of sugar as a function of the concentration of sugar in the juice stream.

$$C_S^{out} = C_S^{in} \cdot (1 - X) \tag{7}$$

$$C_X^{out} = C_X^{in} + C_S^{in} \cdot X \cdot Y_{X/S} \tag{8}$$

$$C_P^{out} = C_P^{in} + C_S^{in} \cdot X \cdot Y_{P/S} \tag{9}$$

Cell recycle in the reactor systems was implemented using a centrifuge that separates the fermented wine stream into a stream of centrifuged wine containing no yeast cells and a stream of yeast cream with 180kg/m³ of cell biomass on a wet basis. The fed-batch system demands the production of 274m³/h of inoculum with 90kg/m³ of cell biomass and the continuous system demands 112m³/h of inoculum with 90kg/m³ of cell biomass. This was

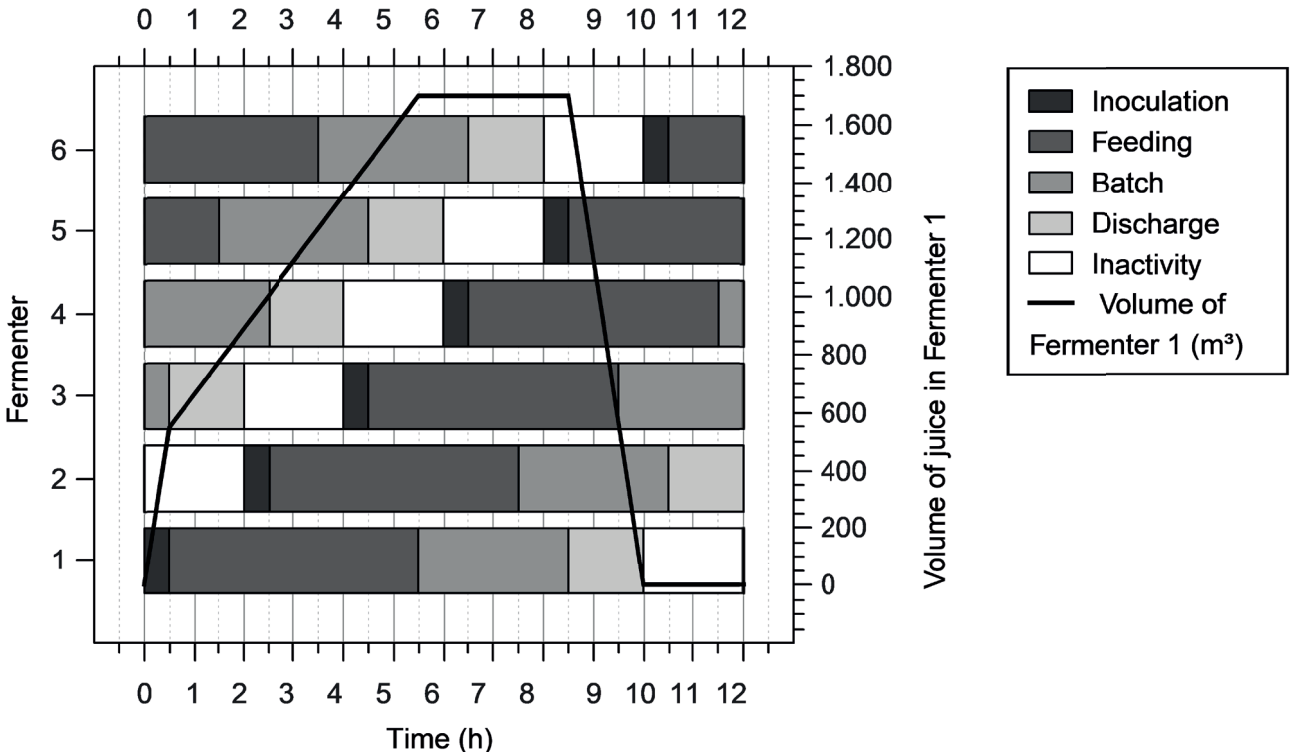

Figure 3. Juice volume profile in Fermenter 1 (continuous line) and behavior of every fermenter (bar chart) during a 12 h cycle.

obtained by mixing equal parts of water and yeast cream stream after a fraction of the yeast cream is purged (ca. 7.5%). This work did not regard either microbial infection or consumption of nutrients other than sugar by the yeast cells during the fermentation, hence the cell treatment was simulated simply as a dilution of yeast cream in water.

A preliminary simulation was made in order to check the adequacy of the parameters in Table 1 to reproduce experimental data from a pilot scale fed-batch fermenter (Martins et al., 2010). The pilot reactor was inoculated with 50 m^3 of yeast cream containing 49 kg/m^3 of cell biomass on a wet basis. It was fed with 77.55 m^3/h of juice containing 18.2% in total sugars during four hours and the entire fed-batch operation lasts nine hours.

The remaining simulations were made assuming industrial-scale fermenters with an input of 575 tonnes of juice per hour to the fermentation system. This value is based on data from a distillery inthe countryside of São Paulo, Brazil. Two alternative configurations for such a distillery were modeled and simulated: one with the system of six parallel fed-batch reactors (dynamic simulation) and one with four continuous reactors (continuous and steady-state simulation). Both configurations were compared to a simulation using a single stoichiometric reactor, in order to assess how well it could reproduce the more complicated systems.

Each one of the fed-batch reactors was inoculated with 548 m^3 of yeast cream containing 90 kg/m^3 of cell biomass. They were fed with 230m^3/h of juice containing 20.0% in total sugars during five hours. At any given moment, either two fermenters or three fermenters will be in the feeding stage, with equal likelihood. That implies that, on average, 575 m^3/h of juice will be fed to the whole system.

In the continuous fermentation system, 575 m^3/h of juice are fed directly to the fermenters. As previously mentioned the volumes of each fermenter were defined by optimization, in order to maximize the production of ethanol.

Sensitivity tests were made for the main kinetic parameters (μ_{max}, k_s and k_i) and the fraction of sugar in the juice. Concentrations of ethanol are expressed on a volume basis (% volume/volume) while concentrations of sugar are expressed in terms of total reducing sugars (TRS) percentage on a mass basis (% mass/mass), as those units are the most common in industrial jargon. Equations 10 and 11 show the conversion factor between those units and the metric system.

$$C_P(\text{kg/m}^3) = 7.893 \cdot C_P(\%\text{vol/vol}) \quad (10)$$

$$C_S(\text{kg/m}^3) = 10.0 \cdot C_S(\%\text{mass/mass}) \quad (11)$$

RESULTS AND DISCUSSION

The results of the preliminary simulation representing the fermentation in a pilot plant are shown in Fig.4, 5 and 6.The simulation results showed that the model fitted fairly well to the experimental data of sugar, cells, and ethanol concentrations.

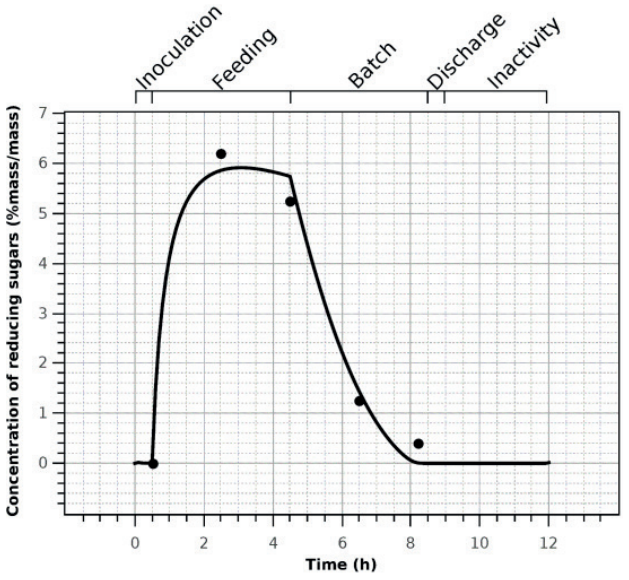

Figure 4. Percentage of total reducing sugars (TRS) on a mass basisduring a full cycle of fed-batch fermentation. Solid line represents model prediction, circles are experimental values (Martins et al., 2010).

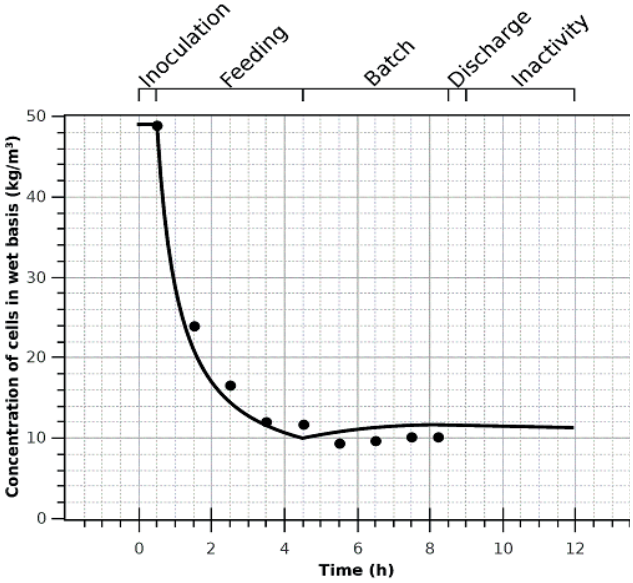

Figure 5. Concentration of cells on a wet basis during a full cycle of fed-batch fermentation. Solid line represents model prediction, circles are experimental values (Martins et al., 2010).

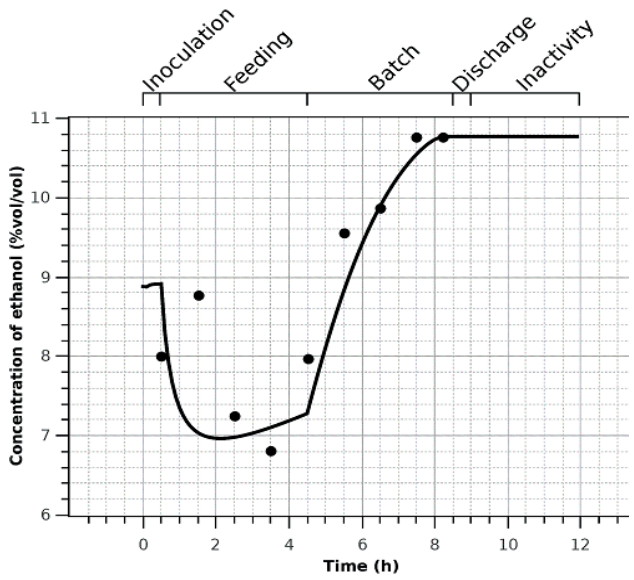

Figure 6. Percentage of ethanol on a volume basis during a full cycle of fed-batch fermentation. Solid line represents model prediction, circles are experimental values (Martins et al., 2010).

The next results discussed in this section refer to the industrial-scale plant. The fed-batch system was implemented as described in the methodology section. Each fermenter held up to 1699 m³ of reactant fluid and their average occupation was 1008 m³. Since six fermenters were used, 6048 m³ of reactant fluid were processed by the system at any given moment, on average.

The continuous system was designed with the constraint that the sum of the volumes of each fermenter should be equal to 6050 m³, which is approximately the same value as the average occupation of the fermenters in the fed-batch system. The volumes of each fermenter were found by a particle-swarm optimization procedure in which the total production of ethanol in the system was optimized. The optimal volumes of the four fermenters are 1816.46 m³, 1854.66 m³, 675.35 m³ and 1703.54 m³ in downstream sequence. Though, it should be noted that the solution found for this optimization problem is on a plateau and many combinations of volumes lead to near-optimal solutions, so there is no guarantee that the values used in this paper correspond to the global maximum.

Tables 2 to 4 show the results of sensitivity tests for the main kinetic parameters of the fermentation model. The output variables deemed relevant to the analysis are the amount of ethanol produced in kg/h, the concentration of ethanol in the wine, on a volumetric basis and the conversion of substrate. The results show very clearly that the model has little sensitivity to the values of μ_{max}, k_s and k_i, since variations of up to 20% in their values are not enough to significantly alter the values of any of these variables.

It was observed that the model is much more sensitive to the concentration of substrate in the juice. Figures 7 and 8 present the values of total ethanol production, ethanol throughput in centrifuged wine and the conversion of substrate as a function of the substrate concentrationin the juice for the fed-batch system (average values) and continuous system, respectively.

Further simulations were made with additional values of sugar concentration in the juice to search for a pattern for the conversion of sugar as a function of the input. The identification of such a pattern would be useful for more accurate stoichiometric approximations for the kinetic-based fermentation models. According to inside information from the distillery which the fed-batch system is based upon, the percentage of reducing sugars in the juice typically ranges from 18% to 22% in mass. The analysis is extended to up to 25%, overshooting those limits. Fig. 9 illustrates the conversion of substrate as a function of the concentration of reducing sugars in the juice (concentrations before the juice is mixed with yeast cream).

Figure 9 shows that, as the content of sugar in the juice rises, the conversion of sugar in both fermenter systems decreases in a linear fashion. Linear regression was used to find equations that fit those trends. For the fed-batch

Table 2. Sensitivity tests for maximum specific cell growth rate (μ_{max}).

	μ_{max}(h^{-1})	0.32	0.36	0.40	0.44	0.48
Fed-batch	Ethanol throughput (kg/h)	59280	59280	59216	59216	59216
	Concentration of ethanol (%vol/vol)	10.72	10.72	10.71	10.71	10.71
	Conversion of sugar	1.0000	1.0000	1.0000	1.0000	1.0000
Continuous	Ethanol throughput (kg/h)	59270	59270	59319	59318	59319
	Concentration of ethanol (%vol/vol)	12.23	12.23	12.24	12.24	12.24
	Conversion of sugar	0.9993	0.9998	0.9999	0.9999	1.0000

Table 3. Sensitivity tests for half-velocity constant (k_s).

	k_S(kg/m³)	0.38	0.43	0.48	0.53	0.58
Fed-batch	Ethanol throughput (kg/h)	59216	59216	59216	59271	59271
	Concentration of ethanol (%vol/vol)	10.71	10.71	10.71	10.72	10.72
	Conversion of sugar	1.0000	1.0000	1.0000	1.0000	1.0000
Continuous	Ethanol throughput (kg/h)	59319	59319	59319	59319	59319
	Concentration of ethanol (%vol/vol)	12.24	12.24	12.24	12.24	12.24
	Conversion of sugar	0.9999	0.9999	0.9999	0.9998	0.9998

Table 4. Sensitivity tests for substrate inhibition constant (k_i).

	k_i(kg/m³)	163.49	183.49	203.49	223.49	243.49
Fed-batch	Ethanol throughput (kg/h)	59216	59216	59216	59280	59271
	Concentration of ethanol (%vol/vol)	10.71	10.71	10.71	10.72	10.72
	Conversion of sugar	1.0000	1.0000	1.0000	1.0000	1.0000
Continuous	Ethanol throughput (kg/h)	59319	59319	59319	59319	59319
	Concentration of ethanol (%vol/vol)	12.24	12.24	12.24	12.24	12.24
	Conversion of sugar	0.9998	0.9998	0.9999	0.9999	0.9999

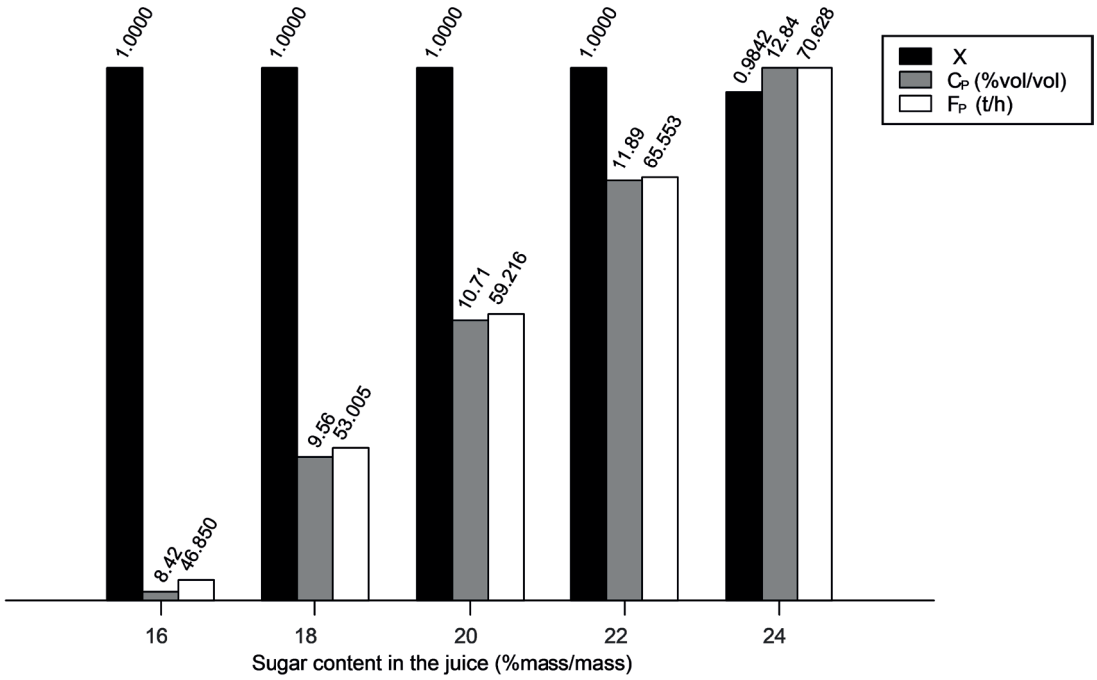

Figure 7. Average values of ethanol throughput (F_p), concentration of ethanol in centrifuged wine (C_p, % volume/volume) and conversion of substrate (X) as a function of the mass percentage of reducing sugars in juice for the fed-batch fermentation system.

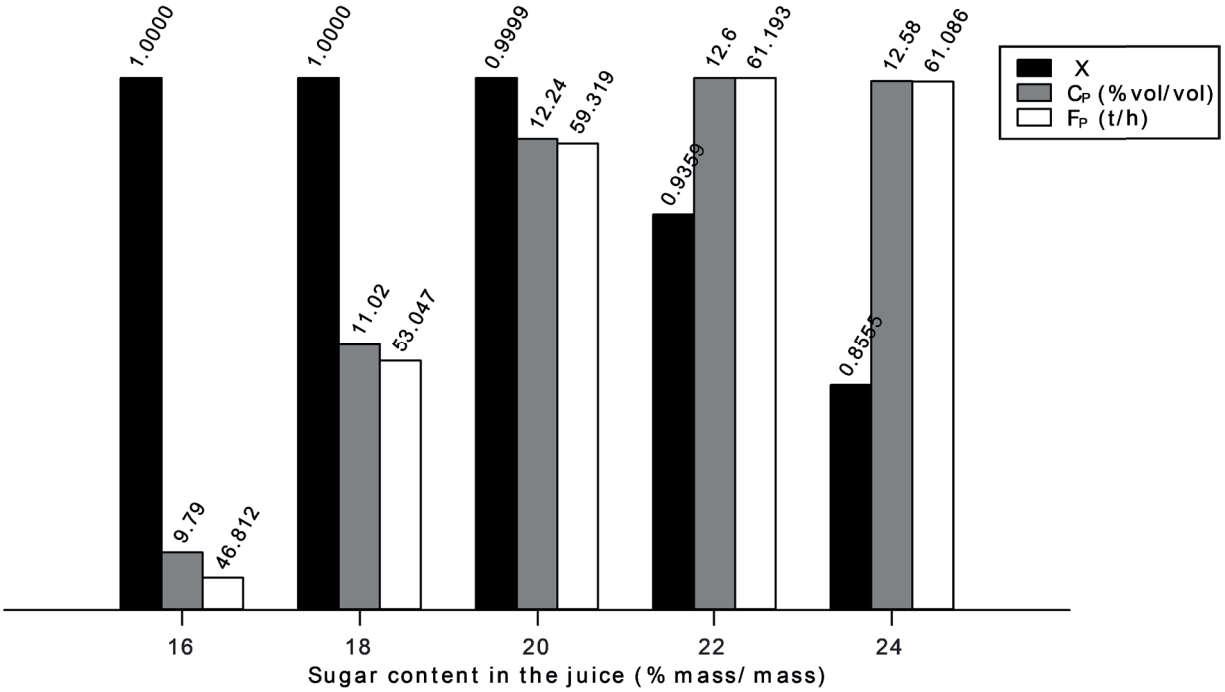

Figure 8. Ethanol throughput (F_P), concentration of ethanol in centrifuged wine (C_P, % volume/volume) and conversion of substrate (X) as a function of the mass percentage of reducing sugars in juice for the continuous fermentation system.

reactor system it is possible to estimate that the conversion of sugar in this particular design is complete for total sugar concentrations of up to 23.1% in the juice. Beyond that concentration, it may be approximated by Equation 12. It should be noted that the concentration of total sugars in the juice doesnot exceed 22% in the industrial facility upon which the fermentation system design was based, hence a stoichiometric model may reproduce the results of a more complex fed-batch simulation with great accuracy for the whole operating range of this design.

The conversion of sugars in the continuous fermenter system is more sensitive to the concentration of sugar in the juice, in comparison to the fed-batch reactor system. It is a foreseeable conclusion, since in the fed-batch system the duration of the batch works as a buffer that conceals any inhibition effect that contributes to decrease the velocity of the reaction. Inasmuch as the steady-state continuous reactor doesnot have such advantage, any change in the attributes of the input stream directly affects the characteristics of the outlet stream. For the fermentation system designed in this paper, the conversion of sugar may be considered complete for reducing sugar concentrations of up to 20.2% in the juice. Beyond that point, it may be estimated by Equation 13.

$$X_{FB} = 1.5874 - 0.0254 \cdot C_S (\%mass/mass) \quad (12)$$

$$X_C = 1.7606 - 0.0376 \cdot C_S (\%mass/mass) \quad (13)$$

It should be obvious to the reader, but it is worth highlighting that Equations 12 and 13 are not at all general rules, they are valid only for the fermentation system designs proposed in this study. Nonetheless, these equations may prove to be of worth for anyone in need of a stoichiometric model that accurately reproduces an industrial design and accounts for potential inhibition effects due to high sugar concentrations in the juice.

Figures 10 and 11 compare the results obtained from a simulation with stoichiometric reactors using the former approximations to simulations using more rigorous fed-batch and continuous models.The stoichiometric model closely reproduces the results obtained from both the fed-batch and continuous models, although the stoichiometric model underestimates the expected concentration of ethanol in the wine for juices with higher concentrations of sugar. However, such high concentrations are unusual in industrial operation.

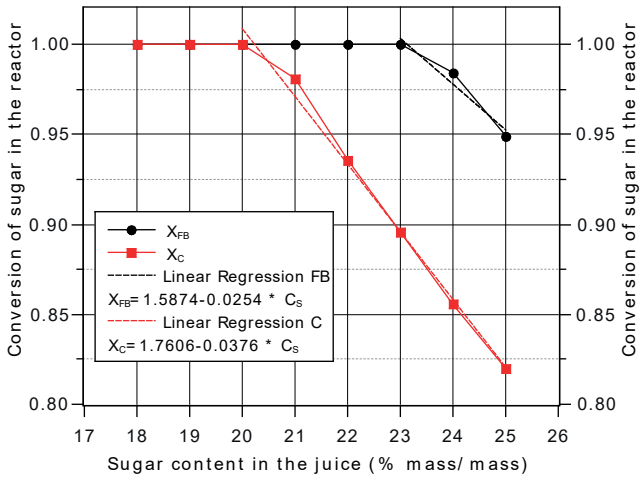

Figure 9. Conversion of substrate as a function of the percentage of sugar in the juice for fed-batch (X_{FB}) and continuous reactors(X_C).

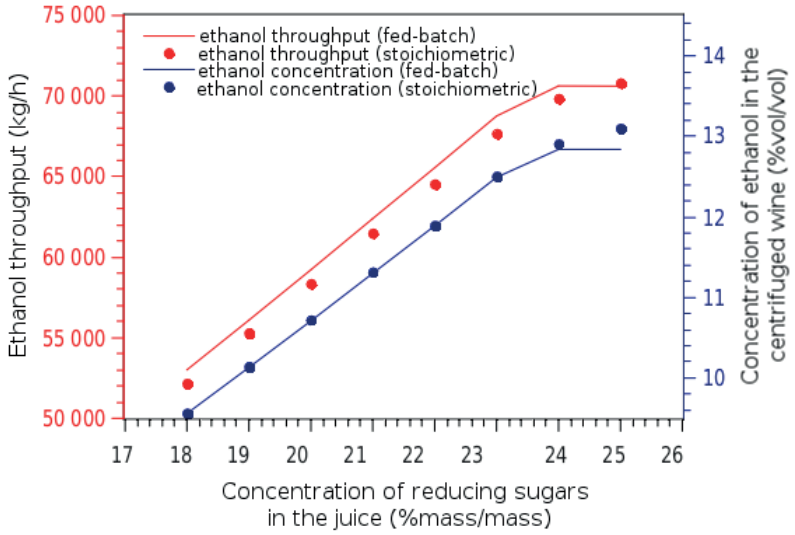

Figure 10. Concentration of ethanol in the wine and throughput of ethanol in a fed-batch fermentation system according to stoichiometric

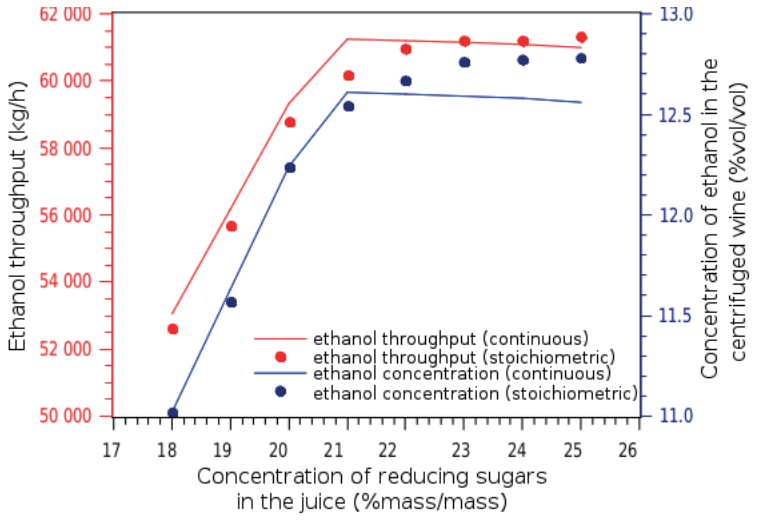

Figure 11. Concentration of ethanol in the wine and throughput of ethanol in a continuous fermentation system according to stoichiometric and steady-state continuous reactor models.

CONCLUSIONS

Stoichiometric fermentation models are preferable in comparison to kinetic based models for plenty of reasons, including ease of development and utilization, faster convergence and the possibility of representing a dynamic process as continuous. All those features make these models more desirable for optimization problems, for example.However, stoichiometric models also have a few drawbacks. One of them is its inability to account for inhibition effects without previous information on the conversion rate of reactant substrate.

In this study, it was found out that the conversion rates for a couple of fermentation system designs can be approximated by linear equations that can be easily incorporated into the stoichiometric model in order to achieve more accurate results. This approximation was practically unnecessary for the fed-batch reactor system discussed in this paper, since the conversion of sugar is virtually complete in the whole range of operation. However, stoichiometric models approximating continuous reactors can be significantly improved by this method, since the conversion rate of sugar within a reactor is much more sensitive to the input concentration of sugar in the case of the continuous reactors than in the case of the fed-batch reactors.

NOMENCLATURE

C_i Concentration of arbitrary component (kg/m^3)

C_i^{in} Concentration of arbitrary component at inlet stream (kg/m^3)

C_i^{out} Concentration of arbitrary component at inlet stream (kg/m^3)

C_P Concentration of ethanol (kg/m^3)

C_P^* Constant of product inhibition (kg/m^3)

C_S Concentration of subtrate(kg/m^3)

C_X Concentration of cells (kg/m^3)

F^{in} Volumetric flow of inlet stream (m^3/h)

F^{out} Volumetric flow of outlet stream (m^3/h)

F_P Ethanol throughput (kg/h)

k_D Rate of cell death (h^{-1})

k_I Constant of substrate inhibition (kg/m^3)

k_S Half-velocity constant (kg/m^3)

r_i Reaction rate of arbitrary component (kg·m^{-3}·h^{-1})

r_P Reaction rate of ethanol (kg·m^{-3}·h^{-1})

r_S Reaction rate of substrate (kg·m^{-3}·h^{-1})

r_X Reaction rate of cells (kg·m^{-3}·h^{-1})

t Time (h)

V Volume occupied by juice (m^3)

X Conversion of sugar (-)

X_{FB} Conversion of sugar in fed-batch reactor (-)

X_C Conversion of sugar in continuous reactor (-)

$Y_{X/S}$ Cell yield coefficient ($kg_{cell}/kg_{substrate}$)

$Y_{P/S}$ Product yield coefficient ($kg_{product}/kg_{substrate}$)

Greek letters

μ Specific cell growth rate (h^{-1}).

μ_{max} Maximum specific cell growth rate (h^{-1}).

ρ Density (kg/m^3)

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