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Backstepping control of the hemicellulose fraction of lignocellulosic biomass in a pretreatment continuous tubular reactor for biofuels production

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Abstract: This paper presents a design of a backstepping control for the hemicellulose fraction existent in lignocellulosic materials used at the first stage of the process of biofuels productions called pretreatment, which is carried out in a continuous tubular reactor. The nonlinear backstepping controller designed regulates the hemicellulose fraction at the output of the process to a desired value. Local asymptotic stability is guaranteed by the proposed Lyapunov functions. The control is successfully validated in simulations employing real data from the continuous tubular reactor process.

Keywords: hemicellulose fraction, backstepping control, lignocellulosic biomass, pretreatment reactor.

1. INTRODUCTION

1.1 Biofuels generation

The increasing demand on energy and the rise of greenhouse gases in the atmosphere lead to the search for new sources of environmentally friendly energy. The development of second generation biofuels from lignocellulosic biomass has many advantages regarding energy and environment, compared with first generation biofuels created from food crops which cause net energy losses, greenhouse gas emission and increased food prices. In addition, the high cost in first generation fuel has contributed with the need of biofuel production from lignocellulosic materials (LCMs), (Alvira et al. (2010)).

Currently, there are many different pathways for producing liquid biofuels such as bioethanol, that are attracting the attention because of the availability and low cost of LCMs as wheat straw and corn stubble. One of these paths is the biochemical procedure that consist of four stages:

- *Pretreatment*: essential step to break down and relocate the robust and recalcitrant structure of the LCMs (composed of cellulose polymers, hemicelluloses, and lignin) in order to increase the accessibility of cellulose and hemicellulose polymers to cellulolytic enzymes and ease the subsequent stages (Koppram et al. (2014)).
- *Enzymatic hydrolysis*: cellulose chains (polymers) are broken through enzymatic reactions to release sugars to be fermented (monomers).
- *Fermentation*: yeasts turn sugar molecules into alcohol molecules producing a mixture of water and alcohol.
- *Separation*: water and contaminants are removed to obtain biofuels with the required purity as to be used as substitutes of fossil fuels.

One of the most commonly used pretreatments is steam explosion, where LCMs undergoes to high pressure steam and temperatures, followed by a violent pressurization. The high temperatures promote acetic acid formation, which partially hydrolyses the biomass, and the depressurization process manages to separate its fibers (González-Figueredo et al. (2015)). The pretreatment stage is crucial in the process of bioethanol production, due to its positive effect on the accessibility to the cellulose and hemicellulose in the LCM matrix for the enzymatic hydrolysis, which directly impacts on the process yields and reducing costs (Mosier et al. (2005)).

1.2 Control of chemical reactors

Control of chemical reactors using backstepping has been studied in previous works. These works mainly center their studies in continuous stirred tank reactors (CSTR), in contrast with this work that studies a continuous tubu-

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lar reactor (CTR) in which the flow behavior is difficult to describe due to complex phenomena for the interaction of the biomass with a screw conveyor (backflow).

Among the contributions for controlling chemical reactor are found the design of a memoryless state feedback backstepping controller for a two-stage CSTR which does not need the precise knowledge of time delays in a recycling system (Hua et al. (2009)). Smyshlyaev and Krstić (2004) designed exponentially convergent observers for a class of parabolic partial differential equations (PPDEs) combined with a backstepping controller to obtain a solution for the boundary output feedback problem, to study the model of heat and mass transfer in an adiabatic tubular reactor. A globally stabilizing boundary feedback control law was proposed by Bošković and Krstić (2002) for the discretization of a nonlinear model that assumes no radial velocity and concentration gradients in a CSTR.

Moreover, Zhao et al. (2017) used the backstepping method to control temperature concentration in a CSTR where the system studied has relative degree higher than one, showing that the feedback system can be written in its error dynamic model form. Biswas and Samanta (2013) presented an adaptive backstepping methodology for controlling a CSTR for polymerization under parametric uncertainty. A hybrid control methodology for a broad class of switched nonlinear systems in strict-feedback form was applied to an adiabatic tubular reactor in (Abdelkarim et al. (2016)).

However, nowadays for the specific case of controlling the hemicellulose fraction of LCMs on a pretreatment CTR to produce biofuels, has not been explored yet using the backstepping method. This method was chosen because of the robustness it provides to systems where the only available measurements are the input and output and there is little or not knowledge of internal states, which is the case of the CTR. Therefore, the main contribution in this paper is the design of a backstepping controller that regulates the hemicellulose fraction existent in the output biomass of the pretreatment process in a CTR, ensuring local asymptotic stability with the Lyapunov functions. The proposed control scheme is successfully validated in simulations employing real CTR data.

This paper is organized as follows: section 2 describes the dynamic model of the variations of the hemicellulose fraction, in section 3 the design procedure is exposed, section 4 shows the simulation results that validates the proposed control and section 5 provides some conclusions.

2. HEMICELLULOSE FRACTION DYNAMIC MODEL

For the case of study in this paper the pretreatment process is carried out in an horizontal pilot-scale continuous tubular reactor (see Figure 1) equipped with steam supply, an external heating jacket, a screw conveyor and a biomass feeding and discharge systems through which the lignocellulosic biomass is subjected to extrusion, autohydrolysis and steam explosion (Cajíca and Sanchez (2018)).

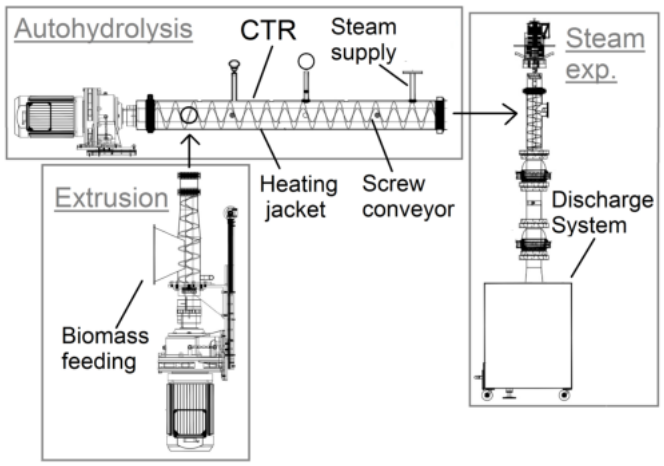


Figure 1. Continuous tubular reactor graphic representation.

The model to describe variations of the hemicellulose fraction in lignocellulosic materials through the CTR is proposed as a set of fourteen dimensionless differential equations

$$\begin{aligned}
\dot{x}_{H_1} &= f_2(x_{H_2} - x_{H_1}) - kx_{H_1} \\
\dot{x}_{H_2} &= f_3(x_{H_3} - x_{H_2}) - kx_{H_2} \\
\dot{x}_{H_3} &= f_4(x_{H_4} - x_{H_3}) - kx_{H_3} \\
&\vdots \\
\dot{x}_{H_{14}} &= u(x_{H_{15}} - x_{H_{14}}) - kx_{H_{14}}.
\end{aligned} \tag{1}$$

where x_{H_i}, f_{i+1}, k, with $i = 1, 2, ..., 14$, are dimensionless hemicellulose fraction, output volumetric flow of the later sub-reactor and $k = k_r\phi$ is a positive constant, respectively; k_r (min^-1) is the reaction rate constant, and $\phi = \frac{v_i}{f_{n_i}}$ is a positive parameter where f_{n_i} (m^3/min) and v_i (m^3) are the nominal volumetric flow and the volume in each sub-reactor. The dimensionless variables are defined in Table 1.

Table 1. Dimensionless variables definition.

Hemicellulose fraction	Volumetric flow	Time
$x_{H_i} = \frac{C_i}{C_0}$	$f_{i+1} = \frac{F_{i+1}}{f_{n_i}}$	$\tau = \frac{t}{\phi}$

System (1) represents divisions of the CTR as CSTR in sub-reactors of identical characteristics connected in series, technique applied in (Cajíca and Sanchez (2018)) to model the CTR mass flow rate and control the residence time, based on the geometric characteristics of the screw conveyor as shown in Figure 2.

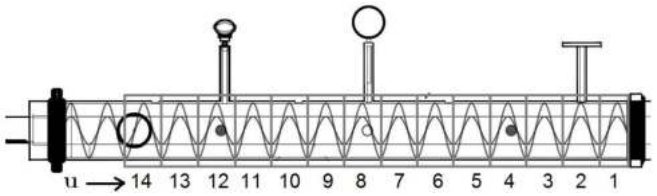


Figure 2. Sub-reactors graphic representation.

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3. CONTROLLER DESIGN

The control scheme is based on the backstepping procedure developed in (Krstic et al. (1992)) using the dimensionless hemicellulose fraction model (1). The objective is to regulate the hemicellulose fraction x_{H_i} in the output biomass of the CTR thus the input volumetric flow of sub-reactor one (f_{15}) is the control input u.

3.1 Backstepping Controller

Despite the division to 14 sub-reactors, the design procedure is recursive so that at its i-th step the i-th-order subsystem is stabilized with respect to a Lyapunov function V_i by the design of a stabilizing virtual control α_i. The feedback control law u is design at the final step.

Step 1: Introducing $z_1 = x_{H_1} - x_{H_{1ref}}$ and $z_2 = x_{H_2} - \alpha_1$ with $x_{H_{1ref}} \in \mathbb{R}^+$, rewriting $\dot{x}_{H_1}$ as

$$\dot{z}_1 = f_2(x_{H_2} - x_{H_1}) - kx_{H_2} \tag{2}$$

and using α_1 as a control to stabilize (2) with respect to the Lyapunov function $V_1 = \frac{1}{2}z_1^2$. Then

$$\dot{V}_1 = z_1(f_2([z_2 + \alpha_1] - x_{H_1}) - kx_{H_1}. \tag{3}$$

Proposing the desired virtual control assuming $z_2 \equiv 0$:

$$\alpha_1 = x_{H_1} + \frac{1}{f_2}(kx_H - k_1 z_1) \tag{4}$$

with this

$$\dot{V}_1 = -k_1 z_1^2 + f_2 z_1 z_2. \tag{5}$$

The term $z_1 z_2$ in $\dot{V}_1$ will be cancelled at the next step. The closed-loop form of (2) with (4) is

$$\dot{z}_1 = -k_1 z_1 + f_2 z_2. \tag{6}$$

Step 2: Introducing $z_3 = x_{H_3} - \alpha_2$, rewriting $\dot{x}_{H_2}$ as

$$\dot{z}_2 = f_3(x_{H_3} - x_{H_2}) - kx_{H_2} - \dot{\alpha}_1 \tag{7}$$

an using α_2 as a control to stabilize the (z_1, z_2)-system (6)-(7) with respect to $V_2 = V_1 + \frac{1}{2}z_2^2$. Then

$$\begin{aligned}\dot{V}_2 = &-k_1 z_1^2 + f_2 z_1 z_2 \dots \\ &+z_2(f_3([z_3 + \alpha_2] - x_{H_2}) - kx_{H_2} - \dot{\alpha}_1).\end{aligned} \tag{8}$$

choosing the desired virtual control assuming $z_3 \equiv 0$:

$$\alpha_2 = x_{H_2} + \frac{1}{f_3}(kx_{H_2} + \dot{\alpha_1} - k_2 z_2 - f_2 z_1) \tag{9}$$

with this

$$\dot{V}_2 = -k_1 z_1^2 - k_2 z_2^2 + f_3 z_2 z_3. \tag{10}$$

The first two terms of $\dot{V}_2$ are negative definite, the third term will be cancelled at the next step. The closed-loop form of (7) with (9) is

$$\dot{z}_2 = -f_2 z_1 - k_2 z_2 + f_3 z_3. \tag{11}$$

Step i: Introducing $z_{i+1} = x_{H_{i+1}} - \alpha_i$, rewriting $\dot{x}_{H_i}$ as

$$\dot{z}_i = f_{i+1}(x_{H_{i+1}} - x_{H_i}) - kx_{H_i} - \dot{\alpha}_{i-1} \tag{12}$$

and using α_i as a control to stabilize the (z_1,..., z_i)-system with respect to $V_i = V_{i-1} + \frac{1}{2}z_i^2$. Then

$$\begin{aligned}\dot{V}_i = &-\sum_{j=1}^{i-1} k_j z_j^2 + f_i z_{i-1} z_i \dots \\ &+z_i(f_{i+1}([z_{i+1} + \alpha_i] - x_{H_i}) - kx_{H_i} - \dot{\alpha}_{i-1}).\end{aligned} \tag{13}$$

Proposing the desired stabilizing function assuming $z_{i+1} \equiv 0$:

$$\alpha_i = x_{H_i} + \frac{1}{f_{i+1}}(kx_{H_i} + \dot{\alpha}_{i-1} - k_i z_i - f_i z_{i-1}) \tag{14}$$

with this

$$\dot{V}_i = -\sum_{j=1}^{i} k_j z_j^2 + f_{i+1} z_i z_{i+1}. \tag{15}$$

The closed-loop form of (12) with (14) is

$$\dot{z}_i = -f_i z_{i-1} - k_i z_i + f_{i+1} z_{i+1}. \tag{16}$$

Step n: Introducing $z_n = x_{H_n} - \alpha_{n-1}$, rewriting $\dot{x}_{H_n}$ as

$$\dot{z}_n = f_{n+1}(x_{H_{n+1}} - x_{H_n}) - kx_{H_n} - \dot{\alpha}_{n-1} \tag{17}$$

Now the feedback control u to stabilize the full z-system with respect to $V_n = V_{n-1} + \frac{1}{2}z_n^2$ is designed. The objective is to make V_n nonpositive:

$$\begin{aligned}\dot{V}_n = &-\sum_{j=1}^{n-1} k_j z_j^2 + f_n z_{n-1} z_n \dots \\ &+z_n(u(x_{H_{n+1}} - x_{H_n}) - kx_{H_n} - \dot{\alpha}_{n-1}).\end{aligned} \tag{18}$$

Finally choosing the control u:

$$u = \frac{1}{x_{H_{n+1}} - x_{H_n}}(kx_{H_n} + \dot{\alpha}_{n-1} - k_n z_n - f_n z_{n-1}) \tag{19}$$

where $(x_{H_{n+1}} - x_{H_n})>0$ and $f_n>0$, and with this

$$\dot{V}_n = -\sum_{j=1}^{n} k_j z_j^2. \tag{20}$$

All terms in $\dot{V}_n$ are negative definite. The closed-loop form of (17) with (19) is

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$$\dot{z}_n = -f_n z_{n-1} - k_n z_n. \tag{21}$$

The overall closed-loop system is:

$$\begin{aligned}
\dot{z}_1 &= -k_1 z_1 + f_2 z_2, \\
\dot{z}_2 &= -f_2 z_1 - k_2 z_2 + f_3 z_3, \\
\dot{z}_3 &= -f_3 z_2 - k_3 z_3 + f_4 z_4, \\
&\vdots \\
\dot{z}_i &= -f_i z_{i-1} - k_i z_i + f_{i+1} z_{i+1}, \\
&\vdots \\
\dot{z}_n &= -f_n z_{n-1} - k_n z_n.
\end{aligned} \tag{22}$$

The stability of the closed-loop system is provided through Lyapunov analysis and is stated in the following theorem.

Theorem 1. Suppose that the control law (19) is applied to system (22). Assuming the term $(x_{H_{n+1}} - x_{H_n}) > 0$ and that the control parameters fulfill $k_i \in \mathbb{R}^+$ with $i = 1, 2, .., n$. Then, the system is locally asymptotically stable.

Proof: To analyze the stability of the closed-loop system (22) α_i is expressed in the z-coordinates. Then, the stability of the equilibrium $z = 0$, where $V_n > 0$ and $V_n = 0$, follows from the fact that the derivative of

$$V_n = V_{n-1} + \frac{1}{2} z_n^2 \tag{23}$$

from (22) is given by

$$\dot{V}_n = -\sum_{j=1}^{n} k_j z_j^2 < 0 \tag{24}$$

where $k_i \in \mathbb{R}^+$ with $i = 1, 2, .., n$. From the above facts we deduct that the Lyapunov function (23) is positive definite and its derivative (24) is negative definite. Moreover, as a consequence of the constraint term $(x_{H_{n+1}} - x_{H_n}) > 0$ in (19) we conclude that the system is locally asymptotically stable.

4. RESULTS

Simulation results of applying the backstepping controller to regulate the hemicellulose fraction of the CTR are presented in this section. Notwithstanding, it is necessary to make some remarks in relation with the physical CTR process:

- To maintain the mass balance of the biomass, the hemicellulose fraction can not surpass levels between 0 - 1, which would represent a normalized value from 0% to 100% of the hemicellulose for any total amount of biomass.
- The input hemicellulose fraction (x_{H_0}) must be 1, this value would be the total of the hemicellulose in the compound of interest.
- The volumetric flow and the volume are positive.

For analyzing the control, the divisions of 7 and 14 sub-reactors are considered regarding real data from the CTR, this is, the reaction rate constant $k_r = 0.055\ min^{-1}$, whose optimal value was determined by Rodríguez (2018) and the nominal volumetric flow $f_{n_i} = 5.56e10^{-5}\ m^3/min$ with $\phi = 1$. The control function for 4, 7 and 14 sub-reactors can be consulted in appendix A.

For the simulations, the initial conditions for x_{H_i} are presented in Table 2 and Table 3 shows the control gains values. It is noticeable from the gain values used in the simulation the need of bigger control gains for the case of 14 sub-reactors than for 7 sub-reactors. The initial value for the volumetric flows is $f_{i+1} = 1$ $(i = 1, 2, .., n)$ that is their maximum value, nevertheless, when $\tau > 1$ $f_{i+1} = f_0$, this means the volumetric flows are updated so that they take the control value (f_0) because internal volumetric flows can not certainly be measured.

Table 2. Initial conditions.

$x_{H_i}(0)$	
x_{H_1}	0.9479
x_{H_2}	0.8985
x_{H_3}	0.8516
x_{H_4}	0.8072
x_{H_5}	0.7651
x_{H_6}	0.7252
x_{H_7}	0.6874
x_{H_8}	0.6516
x_{H_9}	0.6176
$x_{H_{10}}$	0.5844
$x_{H_{11}}$	0.5549
$x_{H_{12}}$	0.5260
$x_{H_{13}}$	0.4968
$x_{H_{14}}$	0.4726

Table 3. Gain values.

Gains	7SR	14SR
k_1	2.5	12.5
k_2	0.01	0.05
k_3	2.5	12.5
k_4	0.01	0.05
k_5	2.5	12.5
k_6	0.01	0.05
k_7	2.5	12.5
k_8		0.05
k_9		12.5
k_{10}		0.05
k_{11}		12.5
k_{12}		0.05
k_{13}		12.5
k_{14}		0.05

On Figures 3 - 4 are exhibited the graphic simulation results of regulating the hemicellulose fraction. A change of 30% less from the value of the initial reference (Table 2) is applied at 20 and 50 units of time for 7 and 14 sub-reactors respectively.

It can be observed how for every number of sub-reactors the hemicellulose is successfully regulated to the reference, the difference is the time the control requires to get the hemicellulose to the reference in steady state (ref_{ss}); in the case of 7 sub-reactors the hemicellulose fraction needs 45 τ to converge but with 14 sub-reactors it needs 140 τ.

Since the volumetric flow can not be negative, the control (f_0) is bounded between 0 - 5, this means that if u<0 then u=0 and if u>5 then u=5. From the physical standpoint, zero means that the reactor is not being fed and five is the maximum nominal flow of biomass allowed at the input of the process. As a consequence of bounding the control function, the changes in the reference must be negatives in order to achieve the right convergence of the hemicellulose fraction.

On Figures 5 - 6 are exhibited the results of applying an error in the model to study the robustness of the control, for this the value of the parameter ϕ is changed to 0.7.

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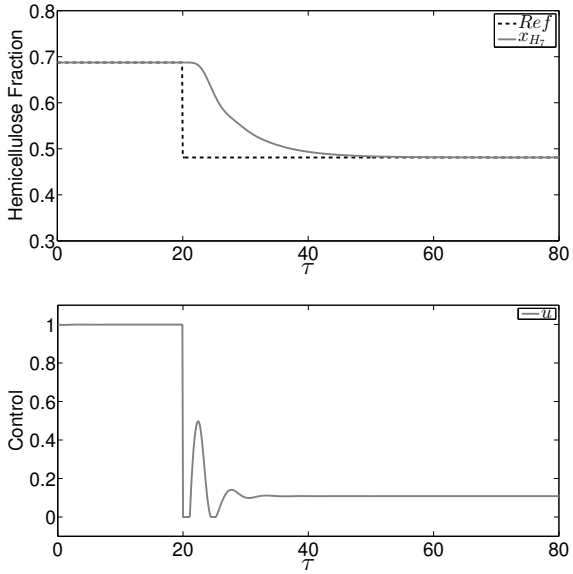


Figure 3. Control for 7 sub-reactors ($ref_{ss} = 0.48$, $u_{ss} = 0.10$).

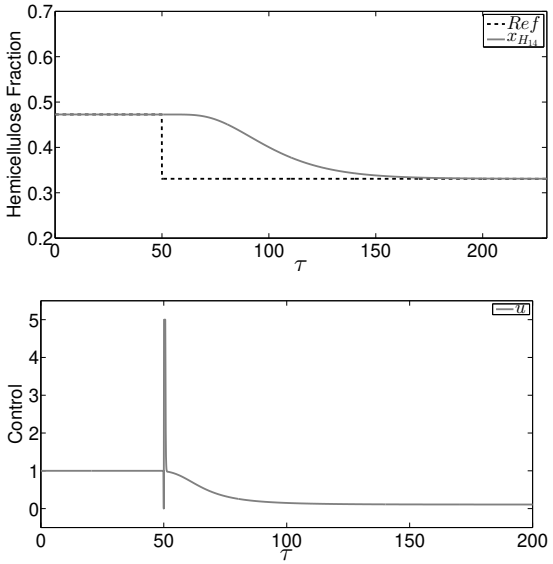


Figure 4. Control for 14 sub-reactors ($ref_{ss} = 0.33$, $u_{ss} = 0.11$).

The hemicellulose fraction converges to the reference for both 7 and 14 sub-reactors and the control in steady state is positive (u_{ss}). Nevertheless, the hemicellulose fraction presents a meaningful oscillation at the beginning of the simulations due to the violent behavior of the control in the first unites of time.

5. CONCLUSIONS

A nonlinear controller based on Lyapunov backstepping design that achieves local asymptotic stabilization to control the hemicellulose fraction of lignocellulosic biomass for the pretreatment process on a continuous tubular reactor has been derived. The simulation study proves that it is possible to regulate the hemicellulose to values under 0.5 which means that a 50% of hemicellulose conversion

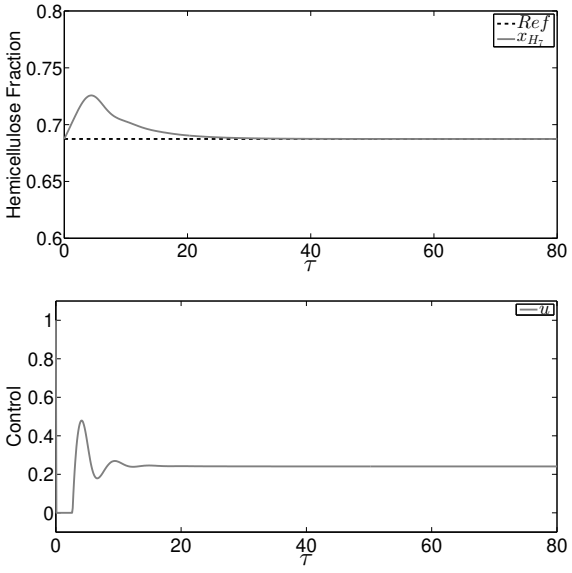


Figure 5. Error in the model for 7 sub-reactors ($ref_{ss} = 0.81$, $u_{ss} = 0.24$).

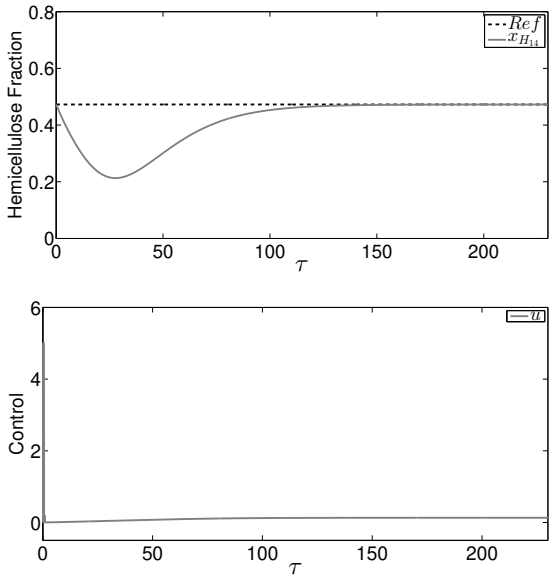


Figure 6. Error in the model for 14 sub-reactors ($ref_{ss} = 0.81$, $u_{ss} = 0.13$).

efficiency can be reached. With backstepping control we have the advantage of ensuring local asymptotic stability through the design, nevertheless, the simulation implementation and the mathematical design become more complicated as the number of sub-reactors rises because this is equivalent to rise the number of step in the design of the control function.

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Nomenclature	
C_0	initial hemicellulose concentration ($\frac{kg}{min}$)
C_i	hemicellulose concentration ($\frac{kg}{min}$)
F_{i+1}	volumetric flow ($\frac{m^3}{min}$)
v_i	volume of sub-reactors (m^3)
f_{n_i}	nominal volumetric flow ($\frac{m^3}{min}$)
k_r	reaction rate constant (min^{-1})
t	time (min)
x_{H_i}	dimensionless hemicellulose fraction
f_{i+1}	dimensionless volumetric flow
τ	dimensionless time

Appendix A. CONTROL LAW FOR 4, 7 AND 14 SUB-REACTORS

The control functions were obtained according to the number of sub-reactors following the design procedure explained on Section 3:

- 4 sub-reactors.

$$u = \frac{1}{x_{H_5} - x_{H_4}}(kx_{H_4} + \dot{\alpha}_3 - k_4 z_4 - f_4 z_3) \qquad (A.1)$$

$$\dot{\alpha}_1 = \dot{x}_{H_1} + \frac{1}{f_2}(k\dot{x}_{H_1} - k_1\dot{z}_1)$$

$$\dot{\alpha}_2 = \dot{x}_{H_2} + \frac{1}{f_3}(k\dot{x}_{H_2} + \ddot{\alpha}_1 - k_2\dot{z}_2 - f_2\dot{z}_1)$$

$$\dot{\alpha}_3 = \dot{x}_{H_3} + \frac{1}{f_4}(k\dot{x}_{H_3} + \ddot{\alpha}_2 - k_3\dot{z}_3 - f_3\dot{z}_2)$$

- 7 sub-reactors.

$$u = \frac{1}{x_{H_8} - x_{H_7}}(kx_{H_7} + \dot{\alpha}_6 - k_7 z_7 - f_7 z_6) \qquad (A.2)$$

$$\dot{\alpha}_1 = \dot{x}_{H_1} + \frac{1}{f_2}(k\dot{x}_{H_1} - k_1\dot{z}_1)$$

$$\dot{\alpha}_2 = \dot{x}_{H_2} + \frac{1}{f_3}(k\dot{x}_{H_2} + \ddot{\alpha}_1 - k_2\dot{z}_2 - f_2\dot{z}_1)$$

$$\vdots$$

$$\dot{\alpha}_6 = \dot{x}_{H_6} + \frac{1}{f_7}(k\dot{x}_{H_6} + \ddot{\alpha}_5 - k_6\dot{z}_6 - f_6\dot{z}_5)$$

- 14 sub-reactors.

$$u = \frac{1}{x_{H_{15}} - x_{H_{14}}}(kx_{H_{14}} + \dot{\alpha}_{13} - k_{14} z_{14} - f_{14} z_{13}) \qquad (A.3)$$

$$\dot{\alpha}_1 = \dot{x}_{H_1} + \frac{1}{f_2}(k\dot{x}_{H_1} - k_1\dot{z}_1)$$

$$\vdots$$

$$\dot{\alpha}_{13} = \dot{x}_{H_{13}} + \frac{1}{f_{14}}(k\dot{x}_{H_{13}} + \ddot{\alpha}_{12} - k_{13}\dot{z}_{13} - f_{13}\dot{z}_{12})$$

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