Optimal operation and control of a batch hydrothermal carbonization reactor

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Abstract: The problem of control and monitoring the operation of a batch hydrothermal (HTC) reactor is addressed, guarantying safe, reliable and efficient operation. The combination of chemical reactors engineering, detectability, passivity, optimality and dynamical inversion tools leads to an event-driven output feedback controller that maximizes the economic profit of the process. The scheme has: (i) an off-line nominal motion generator so that the process is carried out maintaining a compromise between economic profit, speed and effort of control, safety and tolerance against load, measurement and parametric errors, (ii) an event controller that decides the batch end time, guaranteeing the maximum economic profit per unit time, and (iii) a tracking controller that tracks the reactor's motion along an off-line optimized motion. The proposed methodology is applied via numerical simulations of a representative example.

Keywords: Hydrothermal carbonization, batch control, optimal control, material balance control, estimators.

1. INTRODUCTION

Due to concerns and occupations in matter environment and energy, in the last decades interest has grown for designing (Gómez et al., 2020; Peterson and Vogel, 2008) and monitoring kinetic and chemical properties (Funke and Ziegler, 2011) of HTC reactors, leaving aside open problems related to operation and control of this type of reactors for industrial scale applications. In industrial practice, the process design is largely affected by control design therefore, the interaction between both parties leads to integrating models that offers an enriched alternative for the development of such technologies taking into consideration: process knowledge, control theory, optimization and numerical analysis (Seferlis and Georgiadis, 2004). Furthermore, questions and analyzes have been raised about the integrative design as presented by Alvarez et al. (2004), where a joint process and control design for batch processes is proposed using a constructive design and optimizing development with solvability conditions that is designed following passivity, detectability and optimization arguments. Having as starting point these studies, motivates the scope of the present work which consists of developing a model-based joint process-control design methodology for batch HTC reactors with an optimizing stop criterion that maximizes the economic profit of the process.

In this work, the problem of control and monitoring the operation of a batch HTC reactor, guarantying safe, reliable and efficient operation is addressed. The combination of chemical reactors engineering, detectability, passivity, optimality and dynamical inversion tools leads to an estimator-based state material balance controller that maximizes the economic profit of the process. Firstly, the optimal operation is designed by means of iterative application of dynamical inversion (Hirschorn, 1979). Secondly, a non-linear state-feedack tracking (Alvarez et al., 2004) and event optimizing controller is designed following passivity and optimality arguments. Thirdly, a non-linear state estimator of reactive compounds quantities, and, an economic state: utility function, is designed following the process established by Álvarez and Fernández (2009). The combination of tracking and event controllers and state estimator leads to a event-driven output-feedback (OF) controller. The proposed methodology is applied via a numerical simulation to a representative example.

2. CONTROL PROBLEM

The HTC reactors are used for produce biochar from residual biomass by means of a thermochemical process (Basso et al., 2015). We will focus on the simplified solid-solid reaction (1a) that is responsible for producing hydrochar, expressed with mass coefficients generated, taking the molecular weight of biomass (s_B) as reference, and Q_r as the heat released by each biomass mass unit (Felder and Rousseau, 2005). On the other hand, an Arrhenius-type first-order kinetics (1b) (Jatzwauck and Schumpe, 2015) is considered, where $R(M_b, T)$ is the decomposition rate of biomass.

$$s_b C_a H_b O_{c(s)} \rightarrow s_c C_{(s)} + s_a H_2O_{(l)} + Q_r \tag{1a}$$

$$R(M_b, T) = -K_o e^{-\frac{E_a}{R_g T}} M_b := -K(T) M_b \tag{1b}$$

where K_o (or E_a) is the reaction's rate constant (or activation energy), and R_g is the ideal gas constant.

Consider the HTC batch reactor depicted in Fig. 1. with water inlet through valve V_{p1}, wet biomass M_{bh} inlet through valve V_{p2}, heating steam inlet through valve V_{p3}, and pressure relief valve V_c. The system has measurements of reactor (T) and surroundings (T_s) temperatures, and heating steam mass flow (W_s). As an adaptation of the way that an economic state is introduced to determine the optimal (maximum benefit) duration (t_f) of a batch reactive distillation column (Alvarez et al., 2005), let us introduce the analog concept for our present HTC batch reactor case (model parameters are shown in table 1 with their respective values, simbology and description):

$$J(t) = \frac{c_c M_c(t) - c_M M - c_s \int_{t_o}^{t_f} W_s d_\tau}{t + t_d} - c_o \tag{2}$$

$J(t)$ is the utility in time $t = [t_o, t_f]$, defined as the difference between the hydrochar M_c value and the sum of raw material M, heating system and operation costs, where c_c (or c_M) is the hydrochar's value (or raw material's cost) per unit mass, $c_s = c_h Q_v(T)$ is the steam cost per unit mass where c_h is the heating cost per unit heat and $Q_v(T)$ is the latent heat of vaporization, c_o is the operation cost per unit time, t_d is the dead time between batches and $[t_o, t_f]$ is the batch duration with final time t_f.

In time $t_0\,(s)$, water M_{aeo} and wet biomass M_{bho} are loaded to the reactor, where M_{bho} is composed by biomass water M_{ho} and dry biomass (hereinafter called biomass) M_{bo}, with total water loaded amount $M_{ao} = M_{aeo} + M_{ho}$ and loaded biomass amount M_{bo}. Then, in time $0 < t \leq t_f$ the heating steam heats up the mixture from an initial (T_o) to a preset temperature by manipulating the proportional valve V_{p3} to let the biomass M_b degrade into hydrochar M_c, until the utility function $J(t)$ (2) reaches its maximum value at t_f, when $\dot{J} = 0$. The HTC batch reactor model is obtained starting from three mass balances of: biomass, hydrochar and water, and an energy balance, and applying theory of reaction networks and stoichiometric invariants that results in an algebraic-differential system consisting of 2 ordinary differential equations (ODE) (of biomass M_b and temperature T)

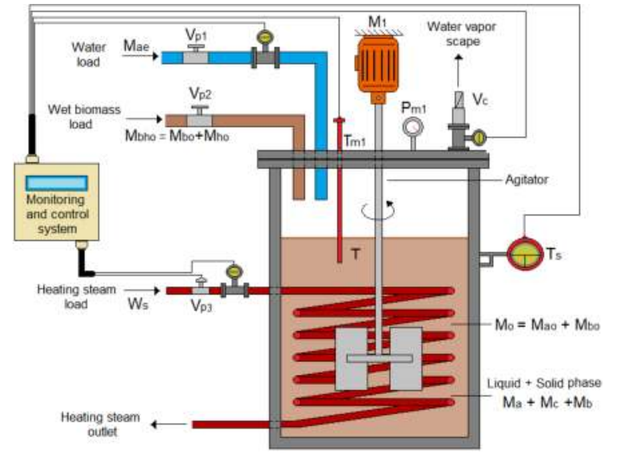

Fig. 1. Hydrothermal Carbonization (HTC) batch reactor

and 2 algebraic equations (of hydrochar M_c and water M_a). This system incorporates an ordinary differential equation of economic performance whose dynamic state is the utility at present time J (2). The combination of the differential algebraic system with the ODE of economic performance results in the following dynamical model (model parameters are shown in table 1):

$$\dot{M}_b = R(T, M_b) := f_{M_b}(M_b, T),\ M_b(0) = M_{bo} \tag{3a}$$

$$\dot{T} = f_T(M_b, T, T_s) + g_T(M_b, T) W_s,\ T(0) = T_o \tag{3b}$$

$$\dot{J} = f_J(M_b, T, J, t) + g_J(t) W_s := f_{Jd}(M_b, T, J, W_s, t),\quad J(0) = -\left(c_M M / t_d + c_o\right) \tag{3c}$$

$$M_c = -s_c M_b + s_c M_{bo} := f_{M_c}(M_b) \tag{3d}$$

$$M_a = M_b(s_c - 1) + M_o - s_c M_{bo} := f_{M_a}(M_b) \tag{3e}$$

$$y = T \tag{3f}$$

where

$$\kappa_1 = s_c \kappa_{ac} - \kappa_{ab}\,,\ \kappa_2 = s_c \kappa_{ac} M_{bo} - \kappa_a M_o$$

$$h(M_b) = \kappa_1 M_b - \kappa_2$$

$$f_T(M_b, T, T_s) = \frac{UA(T_s - T) + K(T) M_b [Q_r + \kappa_1 T]}{h(M_b)}$$

$$g_T(M_b, T) = \frac{Q_v(T)}{h(M_b)}\,,\ g_J(t) = -\frac{c_s}{t + t_d}$$

$$f_J(M_b, T, J, t) = \frac{1}{t + t_d}\left[-J + c_c s_c K(T) M_b\right]$$

(M_b, T, J) is the set of dynamic states, M_b is the amount of biomass, T is the reactor temperature and J is the state utility function. (M_c, M_a) is the set of quasi-static states, M_c (or M_a) is the amount of hydrochar (or water). W_s is the heating steam mass flow, y is the measured output, T_s is the measured ambient temperature, and $[t_o, t_f]$ is the batch duration. In compact notation, the dynamical model (3) is written as follows:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, d, \boldsymbol{p}, t) + \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{p}, t) u := \boldsymbol{f_d}(\boldsymbol{x}, d, \boldsymbol{u}, \boldsymbol{p}, t), \boldsymbol{x}(0) = \boldsymbol{x_o} \tag{4a}$$

$$\boldsymbol{z} = \boldsymbol{S}\,\boldsymbol{x} + \boldsymbol{s}\,\boldsymbol{p},\ y = \boldsymbol{c}\boldsymbol{x}\,,\ t = [t_o, t_f] \tag{4b}$$

where

$\boldsymbol{x} = [M_b, T, J]',\ \boldsymbol{x_o} = [M_{bo}, T_o, J_o]',\ \boldsymbol{z} = [M_c, M_a]',$
$u = W_s,\ d = T_s,\ \boldsymbol{p} = [M_o, M_{bo}]',\ \boldsymbol{c} = [0, 1, 0]$
$\boldsymbol{f}(\boldsymbol{x}, d, \boldsymbol{p}, t) = [f_{M_b}(M_b, T), f_T(M_b, T, T_s), f_J(M_b, T, J, t)]'$
$\boldsymbol{g}(\boldsymbol{x}, \boldsymbol{p}, t) = [0, g_T(M_b, T), g_J(t)]',$
$\boldsymbol{S} = \begin{bmatrix} -s_c & 0 & 0 \\ s_c - 1 & 0 & 0 \end{bmatrix},\ \boldsymbol{s} = \begin{bmatrix} 0 & s_c \\ 1 & s_c - 1 \end{bmatrix}$

System (4) is non-linear and non-autonomous, affine in the control input, where $\boldsymbol{x} \in \mathbb{X} \in \mathbb{R}^3$ is the dynamic state vector, $x_o \in \mathbb{X}$ is the set of initial conditions, $\boldsymbol{z} \in \mathbb{Z} \in \mathbb{R}^2$ is the quasi-static state vector, $[t_o, t_f]$ is the batch duration, $u \geq 0$ is an admissible control, y is the measured output, $d(t) = T_s$ is the exogenous input and $\boldsymbol{p} \in \mathbb{R}^2$ is a parameter vector. The unique solution of system (4) in $[t_o, t_f]$ (since $\boldsymbol{f_d}(\boldsymbol{x}, d, u, \boldsymbol{p})$ is Lipschitz in $(\boldsymbol{x}, d, u, \boldsymbol{p})$ (Elsgotz, 1969)), given the data vector $[\boldsymbol{x_o}, d(t), u(t), \boldsymbol{p}]'$, is the state motion $\boldsymbol{x(t)}$ and its respective quasi-static $\boldsymbol{z}(t)$ and output measured temperature $y(t)$ trajectories:

$$\boldsymbol{x}(t) = \boldsymbol{\tau_x}[t, t_o, \boldsymbol{x_o}, d(t), u(t), \boldsymbol{p}], \tag{5a}$$
$$\boldsymbol{z}(t) = \boldsymbol{\tau_z}[\boldsymbol{x}(t)],\ y(t) = \tau_y[\boldsymbol{x}(t)] \tag{5b}$$

where $\boldsymbol{\tau_x}$ is the state motion transition map and $\boldsymbol{\tau_z}$ (or τ_y) is the quasi-static (or output measured) transition map. Consider the nominal data vector:

$$\bar{\boldsymbol{D}} = [\bar{\boldsymbol{x_o}},\ \bar{y}(t),\ \bar{d}(t),\ \bar{\boldsymbol{p}}]' \tag{6}$$

which applied to system (4) yields the nominal operation:

$$\bar{\boldsymbol{O}} = [\bar{\boldsymbol{x}}(t),\ \bar{\boldsymbol{z}}(t),\ \bar{u}(t),\ \bar{y}(t)],\ t_o \leq t \leq \bar{t_f} \tag{7}$$

that satisfies the particular case of system (4). From now, for simplicity, the explicit dependence on the parameter vector $\boldsymbol{p}$ will be omitted and occasionally used.

Our problem consists in design:
(i) The nominal operation $\bar{\boldsymbol{O}}$ (7) with a suitable compromise between economic profit, batch duration, control effort, and robustness with respect to load, model parameter, and measurement errors.
(ii) A robust output feedback (OF) controller (with state x_c made by the estimate state $\hat{\boldsymbol{x}}$ and an integral state $\hat{\iota}$ of a geometric estimator (Álvarez and Fernández, 2009)):

$$\dot{\boldsymbol{x_c}} = \boldsymbol{f_c}(\boldsymbol{x_c}, d(t), y(t), \bar{y}(t), u),\ \boldsymbol{x_c}(0) = \boldsymbol{x_{co}}, \tag{8a}$$
$$\hat{\boldsymbol{x}} = \boldsymbol{C_e}\boldsymbol{x_c},\ \boldsymbol{x_c} = [\hat{\boldsymbol{x}}, \iota]',\ t = [t_o, t_f] \tag{8b}$$
$$u(t) = \mu[\hat{\boldsymbol{x}}, y(t), \bar{y}(t), d(t)] \tag{8c}$$
$$t_f = \mu_f[\hat{\boldsymbol{x}}, u(t_f), d(t_f), y(t_f), t_f] \tag{8d}$$

which driven by measurements causes the reactor temperature $y(t)$ to offsetlesstly track the nominal temperature $\bar{y}(t)$, and the state motion $\boldsymbol{x}(t)$ tracks up to admissible deviations the nominal state motion $\bar{\boldsymbol{x}}(t)$, by adjusting the steam flow rate u, and on the basis of the state estimate $\hat{\boldsymbol{x}}(t)$, determines the batch duration tracks.

3. NOMINAL OPERATION

Here, the nominal operation (7) is designed via an iterative calibration process based on dynamical inversion (Hirschorn, 1979), guaranteeing practical stability of the state motion, so that the process is carried out with a suitable compromise between economic profit, batch duration, control effort, and robustness with respect to load, model parameter, and measurement errors.

3.1 Stability

Since (4) is a non-autonomous system, the standard definitions of asymptotic stability cannot be formally applied. In this case, these definitions applies to a particular state motion and its deviations caused by data disturbances (Alvarez et al., 2005). Here, the notion of stability of non-autonomous systems is presented based on the definitions of non-local practical stability (Hahn, 1967; LaSalle and Lefschetz, 1961) and ISS stability (Sontag et al., 2004).

For given nominal data

$$\bar{\boldsymbol{D}}_{\boldsymbol{d}} = [\bar{\boldsymbol{x_o}},\ \bar{d}(t),\ \bar{u}(t),\ \bar{\boldsymbol{p}}]' \tag{9}$$

system (4) has unique state motion solution

$$\bar{\boldsymbol{x}}\boldsymbol{(t)} = \boldsymbol{\tau_x}[t, t_o, \bar{\boldsymbol{x_o}}, \bar{d}(t), \bar{u}(t), \bar{\boldsymbol{p}}] \tag{10}$$

For admissibly bounded perturbed data

$$\hat{\boldsymbol{D}}_{\boldsymbol{d}} = \bar{\boldsymbol{D}}_{\boldsymbol{d}} + \tilde{\boldsymbol{D}}_{\boldsymbol{d}}, \tilde{\boldsymbol{D}}_{\boldsymbol{d}} = [\tilde{\boldsymbol{x_o}}, \tilde{d}(t), \tilde{u}(t), \tilde{\boldsymbol{p}}]', |\tilde{\boldsymbol{x_o}}| \leq \delta_o \tag{11a}$$
$$|\tilde{d}(t)| := \delta_d \leq \delta_d^+, |\tilde{u}(t)| := \delta_u \leq \delta_u^+, |\tilde{\boldsymbol{p}}| \leq \delta_p \tag{11b}$$

The motions deviations are

$$\tilde{\boldsymbol{x}}(t) = \hat{\boldsymbol{x}}(t) - \bar{\boldsymbol{x}}(t), \hat{\boldsymbol{x}}(t) = \boldsymbol{\tau_x}[t, t_o, \hat{\boldsymbol{x_o}}, \hat{d}(t), \hat{u}(t), \hat{\boldsymbol{p}}] \tag{12}$$

Definition 1. The nominal state motion $\bar{\boldsymbol{x}}(t)$ (10) over $[t_o, \bar{t_f}]$ is robustly (exponentially) locally or practically stable if the motion deviations (12a) are bounded as

$$\begin{aligned} |\tilde{\boldsymbol{x}}(t)| &\leq a_x e^{-l_x(t-t_o)}\delta_o + b_p\delta_p + b_d\delta_d^+ + b_u\delta_u^+ \\ &\leq a_x\delta_o + b_p\delta_p + b_d\delta_d^+ + b_u\delta_u^+ \\ &= \epsilon_x(\delta_o, \delta_p, \delta_d^+, \delta_u^+),\ \epsilon_x(0,0,0,0) = 0 \end{aligned} \tag{13}$$

The nominal state motion $\bar{\boldsymbol{x}}(t)$ is non-locally practically stable if admissible data disturbances sizes $(\delta_o, \delta_p, \delta_d^+, \delta_u^+)$ produce admissible motion deviation size ϵ_x (LaSalle and Lefschetz, 1961; Hahn, 1967). As we shall see (in Section 3.2, with numerical simulation), the nominal motion $\bar{\boldsymbol{x}}(t)$ of $\bar{\boldsymbol{O}}$ (7) is robustly stable (V. Lakshmikantham, 1990; Alvarez et al., 2005) in the sense that admissible data deviations produce admissible state motion deviations.

3.2 Nominal operation design

Here, the nominal operation is iteratively constructed through dynamical inversion (Hirschorn, 1979), in the sense that, for given inverse data

$$\boldsymbol{D_I} = [\boldsymbol{x_{Io}}, y(t), d(t)] \tag{14}$$

the nominal state motion-input control pair $[\boldsymbol{x}(t), u(t)]$ is uniquely-robustly determined. To construct the dynamical inverse system, take the derivative of the output map (3f) and substitute (3b) to obtain the algebraic equation

$$\dot{y} = f_T(M_b, T, T_s) + g_T(M_b, T)u \tag{15}$$

whose unique solution for $u(t)$ yields the NL SF control

$$u(t) = \frac{\dot{\bar{y}} - f_T[M_{bI}, \bar{y}(t), T_s]}{g_T[M_b, \bar{y}]} := \mu_I[M_{bI}, T_s, \bar{y}(t)] \tag{16}$$

The application of this control to system (4) yields the dynamical inverse

$$\dot{\boldsymbol{x}}_{\boldsymbol{I}} = \boldsymbol{f}_{\boldsymbol{I}}\{\boldsymbol{x}_{\boldsymbol{I}}, \bar{y}(t), d(t), \mu_I[\boldsymbol{x}_{\boldsymbol{I}}, d(t), \bar{y}(t)]\} \quad (17a)$$

$$u(t) = \mu_I[\boldsymbol{x}_{\boldsymbol{I}}, d(t), \bar{y}(t)],\ \boldsymbol{x}_{\boldsymbol{I}}(0) = \boldsymbol{x}_{\boldsymbol{Io}} \quad (17b)$$

where

$$\boldsymbol{x}_{\boldsymbol{I}} = [M_b, J]',\ \boldsymbol{f}_{\boldsymbol{I}} = [f_{M_b}, f_{Jd}]'$$

In control literature (17a) is called the zero-dynamics and (17b) the associated NL SF control (Alvarez et al., 2004). The unique state motion solution of system (17) and its corresponding quasi-static trajectory are:

$$\boldsymbol{x}_{\boldsymbol{I}}(t) = \boldsymbol{\tau}_{\boldsymbol{x}_{\boldsymbol{I}}}[t, t_o, \boldsymbol{x}_{\boldsymbol{Io}}, d(t), \bar{y}(t)],\ \boldsymbol{z}_{\boldsymbol{I}}(t) = \boldsymbol{\tau}_{\boldsymbol{zI}}[\boldsymbol{x}_{\boldsymbol{I}}(t)] \quad (18)$$

To tune the inverse, the prescribed output temperature trajectory is set

$$\bar{y}(t) = (\bar{T} - T_o)(1 - e^{-\lambda t}) + T_o \quad (19)$$

where $\bar{T}$ is the target temperature and λ is an adjustable speed parameter, to be chosen so that an suitable compromise between economic profit, speed, robustness and control effort is attained through an iterative procedure where the initial guess is refined. While the relative degree equal to one condition is met because $h(M_b) > 0$ (3), the robust passivity (stability) of the nominal inverse must be assessed with numerical simulation in presence of typical model and data errors.

4. STATE-FEEDBACK CONTROL

Here, assuming the state $\boldsymbol{x}(t)$ is known, a NL SF tracking controller is constructed according to the design procedure for batch chemical processes (Alvarez et al., 2004). The enforcement of the output tracking dynamics

$$\dot{T} = -k_c[T - \bar{y}(t)],\ T(0) = \bar{y}(t) = \bar{y_o} \quad (20)$$

to the reactor (4) leads to the algebraic equation:

$$f_T(M_b, T, T_s) + g_T(M_b, T)u = \dot{\bar{y}} - k_c[T - \bar{y}(t)] \quad (21)$$

whose unique solution for $u(t)$ yields the NL SF tracking controller

$$u(t) = \frac{\dot{\bar{y}} - k_c[y(t) - \bar{y}(t)]}{g_T(M_b, y)} - \frac{f_T(M_b, y, T_s)}{g_T(M_b, y)} := \mu[\boldsymbol{x}, d(t), y(t), \bar{y}(t)] \quad (22)$$

The event controller, that determines the batch final time t_f, is derived from the economic state as follow

$$t_f = \mu_f[\boldsymbol{x}, y(t_f), d(t_f), u(t_f), t_f] \ni f_{Jd}[\boldsymbol{x}, y(t), u(t), t] = 0 \quad (23)$$

where $f_{Jd}[\boldsymbol{x}, y(t), u, t]$ is the batch stop criterion, which detects that $J(t)$ has reached a maximum when $\dot{J} = 0$. The event (23) and tracking (22) NL SF controllers applied to the reactor (4) yields the closed-loop dynamics

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, d) + \boldsymbol{g}(\boldsymbol{x})\mu(\boldsymbol{x}, d, y, \bar{y}),\ \boldsymbol{x}(0) = \boldsymbol{x_o} \quad (24a)$$

$$u = \mu[\boldsymbol{x}, d, y(t), \bar{y}(t)],\ t_f = \mu_f[\boldsymbol{x}, y(t_f), d(t_f), u(t_f), t_f] \quad (24b)$$

From the robust passivity of the the dynamical inversion, the closed loop robust motion stability property follows.

5. OUTPUT-FEEDBACK CONTROL

Here, the NL OF controller (8) that combines the SF controller (24) and a geometric state-estimator (Álvarez and Fernández, 2009) is addressed, considering that $\boldsymbol{x}(t)$, which was previously known, is now to be estimated.

5.1 State estimation

Our problem consists in infering the unknown dynamic states: biomass M_b and utility function J, and, the quasi-static states: hydrochar mass M_c and water mass M_a, from knowledge of the data: $[\boldsymbol{x_o}, d(t), y(t), u(t)]$.
From (4) the observability map is given by:

$$o(\boldsymbol{x}, d, u) = [y, \dot{y}]' = \{T, f_T(\boldsymbol{x}, d, u)\}' \quad (25)$$

The Jacobian of $o(\boldsymbol{x}, d, u)$ leads the NL estimation matrix:

$$\boldsymbol{O}(\boldsymbol{x}, d, u) = \begin{bmatrix} 0 & 1 \\ f_{M_b e}(\boldsymbol{x}, d, u) & f_{Te}(\boldsymbol{x}, u) \end{bmatrix} \quad (26a)$$

$$f_{M_b e}(\boldsymbol{x}, d, u) = \frac{\partial f_T(\boldsymbol{x}, d, u)}{\partial M_b},\ f_{Te}(\boldsymbol{x}, u) = \frac{\partial f_T(\boldsymbol{x}, d, u)}{\partial T} \quad (26b)$$

It was found that along the nominal motion $\bar{\boldsymbol{x}}(t)$ the observability matrix: i) is robustly invertible for $t = [t_o, t_s]$, with t_s being approximately one quarter of the batch duration t_f, and ii) is almost singular for $t = (t_s, t_f]$. Consequentely: (i) the nominal motion $\bar{\boldsymbol{x}}(t)$ is robustly detectable along $[t_o, tf]$, and (ii) the measurement injection must be applied only along $[t_o, t_s]$, with setting of injection to no injection mechanism at t_s where $\boldsymbol{O}(\boldsymbol{x}, d, u)$ becomes singular within a prescribed tolerance ϵ_e, according to the injection-no injection switcher

$$P(t - t_s) = \begin{cases} 0, & if\ \ det[\boldsymbol{O}(\boldsymbol{x}, d, u)] < \epsilon_e \\ 1, & if\ \ det[\boldsymbol{O}(\boldsymbol{x}, d, u)] \geq \epsilon_e \end{cases} ,t = [t_o, t_f] \quad (27)$$

where H is Heaviside step function. Thus, the geometric estimator is given by

$$\dot{\hat{\boldsymbol{x}}} = \boldsymbol{f}(\hat{\boldsymbol{x}}, d) + \boldsymbol{g}(\hat{\boldsymbol{x}}) + P(t)\{\boldsymbol{\gamma_p}(\hat{\boldsymbol{x}}, d, u)(y - \boldsymbol{c}\hat{\boldsymbol{x}}) + \boldsymbol{\gamma_\iota}(\hat{\boldsymbol{x}}, d, u)\hat{\iota}\}\ ,\ \hat{\boldsymbol{x}}(0) = \hat{\boldsymbol{x_o}} \quad (28a)$$

$$\dot{\hat{\iota}} = K_\iota[y - \boldsymbol{c}\hat{\boldsymbol{x}}],\ \hat{\iota}(0) = \hat{\iota}_o,\ t = [t_o, t_f] \quad (28b)$$

$$\hat{\boldsymbol{z}} = \boldsymbol{S}\,\hat{\boldsymbol{x}} + \boldsymbol{s},\ \hat{y} = \boldsymbol{c}\hat{\boldsymbol{x}} \quad (28c)$$

where

$$\boldsymbol{\gamma_p}(\hat{\boldsymbol{x}}, d, u) = \begin{bmatrix} \boldsymbol{O}^{-1}(\hat{\boldsymbol{x}}, d, u)\boldsymbol{K_o} \\ 0 \end{bmatrix}, \boldsymbol{K_o} = \begin{bmatrix} 2\zeta\omega \\ \omega^2 \end{bmatrix},$$

$$\boldsymbol{\gamma_\iota}(\hat{\boldsymbol{x}}, d, u) = \begin{bmatrix} \boldsymbol{O}^{-1}(\hat{\boldsymbol{x}}, d, u)K_\iota\boldsymbol{\pi} \\ 0 \end{bmatrix}, \boldsymbol{\pi} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, K_\iota = \omega^3$$

$$\zeta \approx [1, 3], \omega = \eta_\omega \omega_n$$

$\hat{\boldsymbol{x}} = [\hat{\boldsymbol{x}}_{\boldsymbol{\iota}}, \hat{x}_\nu]$ is the dynamic estimated vector where $\hat{\boldsymbol{x}}_{\boldsymbol{\iota}} = [\hat{M}_b, \hat{T}]$ (or $\hat{x}_\nu = \hat{J}$) is the innovated (or non-innovated) state vector, $\hat{\iota}$ is an integral action that eliminates the output mismatch, K_o (or K_ι) is the estimation gain matrix (or integral action gain), η_ω is a convergence speed parameter, t_s is the natural settling time, ω (or ζ) is the characteristic frequency (or damping factor) of the quasi

Table 1. Case example model parameters

Sym.	Description	Value	Unit
κ_a	Specific heat of liquid water	4.18	$\frac{KJ}{Kg\,^\circ K}$
κ_{ab}	Difference between specific heat of liquid water and biomass	2.78	$\frac{KJ}{Kg\,^\circ K}$
κ_{ac}	Difference between specific heat of liquid water and hydrochar	2.92	$\frac{KJ}{Kg\,^\circ K}$
κ_{av}	Difference between specific heat of liquid water and water steam	2.34	$\frac{KJ}{Kg\,^\circ K}$
$Q_v(T)$	Latent heat of vaporization	$f(T)$	$\frac{KJ}{Kg}$
M	Total mass	10000	Kg
U	Heat transport to ambient coefficient	2.5	$\frac{W}{^\circ K m^2}$
A	Reactor surface exchange area	19.981	m^2
s_c	Mass stoichiometric coefficient of hydrochar	$\frac{72}{162}$	-
Q_r	Exothermic heat per unit mass	$\frac{100}{162}$	$\frac{KJ}{Kg}$
E_a	Activation energy	26.25	$\frac{KJ}{mol}$
K_o	Reaction's rate constant	0.1516	$\frac{1}{s}$

LNPA output estimation error dynamics (Álvarez and Fernández, 2009), ω_n is the natural reactor frequency. The presence of the commuter $P(t)$ ensures the non-local practical convergence of the augmented state estimate $(\hat{\boldsymbol{x}}, \hat{\iota})$ towards the augmented state $(\boldsymbol{x}, \iota)$ around the nominal one $(\bar{\boldsymbol{x}}, \bar{\iota})$, provided the damping factor (ζ) and the characteristic frequency (ω) are adequately chosen with the correct parameter tuning through numerical simulation. The stability of $\hat{x}_\nu(t)$ follows from stability of the inverse state motion (18a) and its estimation performance is to be assessed through numerical simulation.

5.2 Output-feedback control

The implementation of the SF tracking-event controller (24) with a structurally compatible NL geometric state estimator (28) yields the NL OF tracking-event controller

$$\begin{aligned}\dot{\hat{\boldsymbol{x}}} =& \boldsymbol{f}(\hat{\boldsymbol{x}}, d) + \boldsymbol{g}(\hat{\boldsymbol{x}})\mu[\boldsymbol{x}, d, y, \bar{y}] \\ &+ P(t)\{\boldsymbol{\gamma_p}(\hat{\boldsymbol{x}}, d, \mu[\boldsymbol{x}, d, y, \bar{y}])(y - \boldsymbol{c}\hat{\boldsymbol{x}}) \\ &+ \boldsymbol{\gamma_\iota}(\hat{\boldsymbol{x}}, d, \mu[\boldsymbol{x}, d, y, \bar{y}])\hat{\iota}\}\,,\ \hat{\boldsymbol{x}}(0) = \hat{\boldsymbol{x}}_{\boldsymbol{o}}\end{aligned} \quad (29a)$$

$$\dot{\hat{\iota}} = K_\iota[y - \boldsymbol{c}\hat{\boldsymbol{x}}],\ \hat{\iota}(0) = \hat{\iota}_o,\ t = [t_o, t_f] \quad (29b)$$

$$\hat{\boldsymbol{z}} = \boldsymbol{S}\,\hat{\boldsymbol{x}} + \boldsymbol{s}\,\boldsymbol{p},\ u = \mu[\boldsymbol{x}, d, y, \bar{y}] \quad (29c)$$

$$t_f = \mu_f[\boldsymbol{x}, y(t_f), d(t_f), u(t_f), t_f] \quad (29d)$$

The closed-loop motion stability is ensured with η_ω tuned (5-10 times) faster than the dominant (biomass) dynamics and $\zeta > 1$.

6. APPLICATION EXAMPLE

Case example: Let us recall the HTC batch reactor (4). The 12 model parameters used for the present case are shown in table 1 with their respective values and units. $Q_v(T)$ was obtained by third order polynomial regression from latent heat of vaporization of water at saturation pressure tables for a temperature range between $(273 - 573\,^\circ K)$ that yields the algebraic function: $f(T) = -0,000024T^3 + 0,023029T^2 - 9,848226T + 3958,647031$.

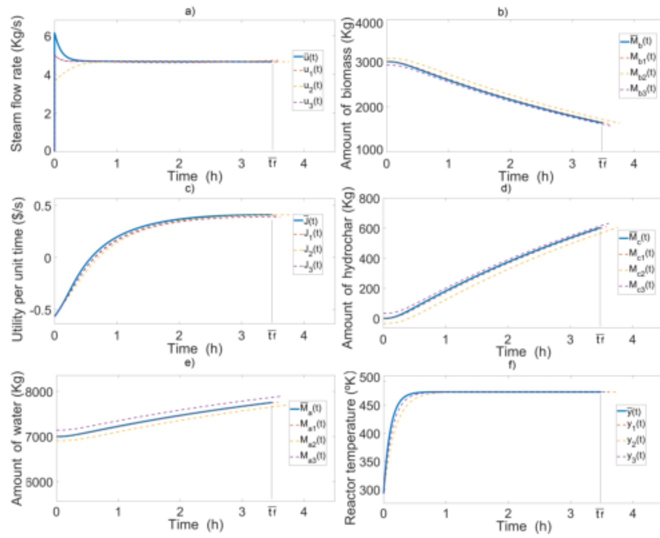

Fig. 2. Nominal operation (continous) with iterative application of the dynamical inversion (discontinous). (a) Control effort, (b,c)dynamic states, (d,e)quasi-static states, (f)measured output.

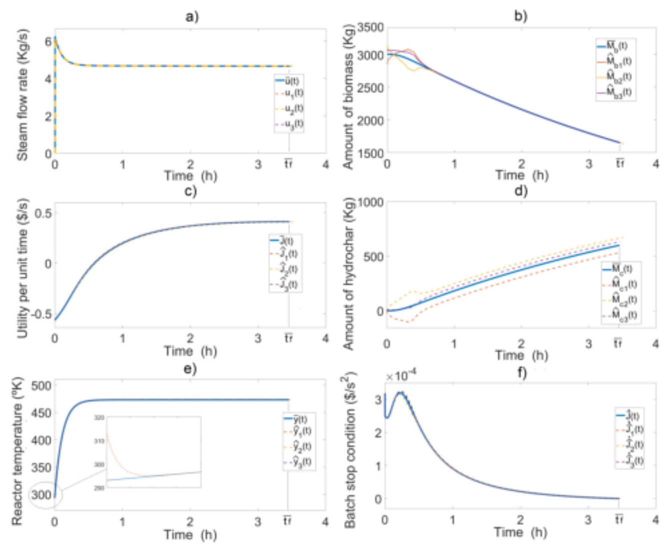

Fig. 3. Closed-loop NL OF controller noiseless behavior for different $\hat{\boldsymbol{x}}_{\boldsymbol{o}}$. (a)Control effort, (b,c)dynamic states, (d)quasi-static state, (e)measured output, (f)batch stop criterion.

• Nominal operation: The application of the design structure (17) with $\bar{T} = 473\,^\circ K$, $T_o = 293\,^\circ K$ and $\lambda = 0.002$ yields the nominal operation shown in Figure 2 with $\bar{t_f} = 3.4\,h$ when utility per unit time is maximum. Figure 2 shows the application of four iterations of the dynamical inverse, were the fourth tray (continuous line) is the nominal motion.

• Closed-loop behavior: The application of the OF control (29) with $k_c = 0.01$, $\omega = 0.0064\,s^{-1}$, $\eta_\omega = 10$, $\zeta = 1.5$ and $\epsilon_e = 0.015$ yields the closed-loop noiseless behavior shown in Figure 3 with $(t_s, t_f) = (0.8, 3.4)h$, with a negligible

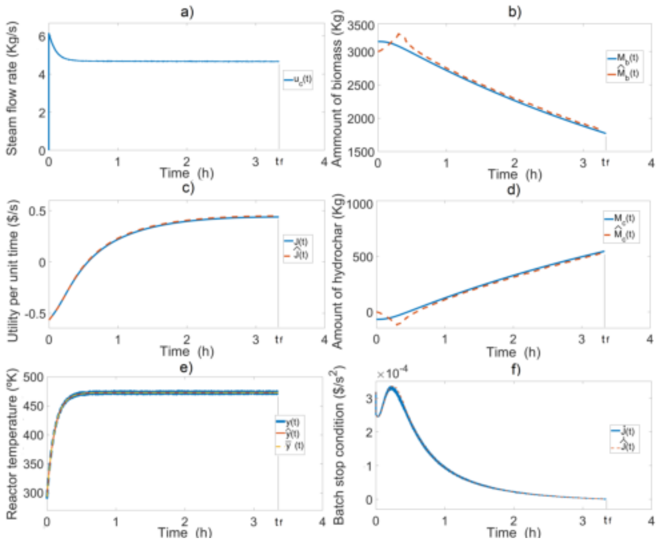

Fig. 4. Closed-loop NL OF controller robustness in presence of admissible errors. (a) Control effort, (b,c)dynamic states, (d) quasi-static state, (f)measured output, (g)batch stop criterion.

variation of $\pm 5\,min$, which means an optimal performance of the event controller, furthermore the estimated dynamical state motion $\hat{\boldsymbol{x}}(t)$ tends to the nominal motion $\bar{\boldsymbol{x}}(t)$ with and acceptable error and the tracking control action results in the measured temperature output $y(t)$ tracking the nominal output temperature $\bar{y}(t)$ instantly as shown in Figure 3e. The closed-loop NL OF controller presents a robust behavior as shown in figure 4, in presence of real and acceptable load and model parameter errors, and measured reactor and ambient temperature noise, with Gaussian (zero-mean and amplitude of $0.5\,{}^{\circ}K$) random temperature errors added every second, and the estimator initialized with $\pm 5\,\%$ load error, which means that the state motion $\hat{\boldsymbol{x}}(t)$ is non-locally practically stable.

7. CONCLUSIONS

The problem of control and monitoring the optimized operation of a batch hydrothermal (HTC) reactor has been addressed within a constructive framework by combining passivity, optimality and detectability notions. The proposed methodology has solvability conditions and systematic control construction with a simple tuning scheme. The optimality-based event control proved to be a successful adjustable criterion to define the batch final time based in operation, dead time and raw material costs, and hydrochar value. The nominal operation was successfully tracked by the application of a event-based NL OF controller and the monitoring system robustly estimates the amounts of chemical species as well as the economic state. The robust functioning of the control-monitoring scheme was positively verified with numercial simulation. This result is a point of departure for future work aimed to formally proof robust convergence functioning within a NL non-autonomous final time motion stability framework (V. Lakshmikantham, 1990), including upper control and estimation limits due to measurement noise (Alvarez et al., 2005).

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