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Suitable temperatures and reaction heats estimation within an intensified heat exchanger/reactor

Xue Han 1,2 , Mondher Farza 2 , Mohammed M'Saad 2 , Boutaib Dahhou 3

Abstract— This paper addresses the estimation problem of temperatures and reaction heat within an intensified heat exchanger/reactor (HEX reactor) from the available temperature measurements, namely the input and output temperature measurements. This estimation is performed by a high gain cascade observer incorporating a suitable saturation function to deal with the peaking phenomena which will referred to as a suitable high gain cascade observer (SHGCO). This observer has been developed from a recent research activity devoted to the high gain observer engineering features bearing in mind promising modelling results of the HEX reactor involving a cascade of sub-reactor models. The effectiveness of the proposed SHGCO has been illustrated throughout relevant simulation results with particular emphasis on the estimation accuracy and the remarkable peaking phenomenon reduction during transition periods.

I. INTRODUCTION

Remarkable attention has been paid to the process intensification technologies over the last decades leading thereby to significant r eductions i n p rocess s ize a nd e nergy consumption, namely the HEX reactor which is obtained by combining a heat exchanger with a chemical reactor. This hybrid plant is nothing but a plug-flow reactor with multifunctional capabilities as pointed out in [1], [2] and [3]. In addition to its exceptional thermal and hydrodynamic performance, the HEX reactor is designed to facilitate chemical reactions under optimized operating conditions. These conditions involve elevated temperatures and concentrations, aiming to expedite reaction kinetics and minimize solvent usage.

It is however worth mentioning that the HEX reactor safe operation is still a challenging problem in view of the lack of cheap and readily available instrumentation for real-time monitoring. This problem has been essentially addressed using appropriate state observers to perform an admissible estimation of the state variables as well as reaction heats in real-time ([4], [5], [6] and [7]). Five contributions have been made to deal with specific s afe o peration problems by properly designing an observer to this end. The first contribution is an adequate observer which can be viewed as a virtual sensor for the actuator system used for the HEX reactor, leading thereby to crucial actuator estimation performance insights ([9]). The second contribution is an extended high gain observer performing a joint estimation of the unmeasurable reactor temperatures and heat transfer

parameters ([9]). The third contribution is devoted to a set of interval observers providing an admissible estimation of the reactor temperature together with some of its specific parameters ([10]). The fourth contribution consists of a comparison study of the performances of five observers that have been proposed for the HEX reactor ([11]). The fifth contribution is an adaptive observer for fault diagnosis and fault-tolerant control ([12]). The involved adaptive observer is essentially used for parameter estimation purposes.

In all the above contributions, the observers of the HEX reactor have been designed using a simple model of the reactor for the required accuracy. An appropriate cascade modeling approach of the HEX reactor has been recently in [13] assuming that the reactor can be properly decomposed in a cascade of sub-reactors that can be reasonably modeled by a simple model. The involved model has been already used in [18] to provide a fault diagnosis approach based on distributed adaptive observers bearing in mind recent results on the high gain observer design ([14], [15], [16] and [17]). The adaptive observers are used to provide an admissible joint estimation of the state variables as well as some key parameters as a suitable parametrization from a specific set of temperature measurements. These measurements are not available in real world life and hence the challenging intensified HEX reactor safe operation problem is still open.

This paper provides a SHGCO for the HEX reactor, using only the available temperature measurements while providing both state and parameter estimations at the same time. Of particular interest, a suitable saturation function has been incorporated in the cascade observer design to alleviate its performances during its transient behavior thereby reducing the intrinsic peaking phenomenon of the high gain principle. The paper is organized as follows. The SGHCO problem is concisely stated in section IV throughout the appropriate modeling of the HEX reactor. The proposed SHGCO is comprehensively presented in section III with particular emphasis on its implementation features. Probing simulation results are given in section IV to demonstrate the effectiveness of the proposed SHGCO. Some concluding remarks are given in section V while emphasizing the perspective of the paper.

II. OBSERVER DESIGN MODEL

The ultimate motivation of this paper consists in providing an admissible estimation of the temperatures and reaction heats within an intensified HEX reactor. And since the estimation process performance is closely related to the considered design model, a particular effort has been paid to the modeling approach pursued in [3] to elaborate a relevant

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design model for suitable estimation under consideration. Such a modeling approach is essentially based on mass and energy balances bearing in mind the observability requirements. Two key features of this modeling approach are worth to be pointed out.

A. Mathematical modeling of the HEX reactor

The HEX reactor is composed of three process plates and four utility plates embedded inside square cross-section channels as shown in figure 1. Reactants are injected into the process channels and the chemical reactions take place within them, while water is injected into the utility channels to either heat the reactants or dissipate reaction heat as soon as possible. The heat transfer media is called the plate wall.

Fig. 1: Physical structure of the HEX reactor: (a) process plate; (b) utility plate; (c) HEX reactor

In a prior study [13], we presented a comprehensive modeling process for the HEX reactor, incorporating a non-linear numerical model consisting of 255 calculation modules. This model was designed to explore the heat exchange characteristics and hydrodynamics of the internal liquid. However, the complexity of the proposed model poses challenges in designing observers or control laws for subsequent applications in fault diagnosis and fault-tolerant control. Balancing the trade-off between accuracy and model complexity, the HEX reactor is conceptualized as a tube comprising a series of interconnected sub-reactors, as shown in figure 2. The fluid is injected into the process plate and the utility plate in co-current, and the plate wall is sandwiched between them.

Fig. 2: Simplified structure of a HEX reactor.

The thermal and hydrodynamic characteristics of the HEX reactor are investigated using a set of thermocouples positioned on the process plate. Utilizing the thermocouple locations as a reference, the HEX reactor model is divided into seven units, each with distinct volumes. Each reactor unit comprises three components: a process cell, a utility cell, and a plate wall cell. Heat exchange takes place vertically between adjacent cells, specifically, from the process cell to the plate wall cell and from the utility cell to the plate wall cell. Notably, heat loss to the surroundings is neglected in this configuration.

Of practical interest, the model validation has been performed with an intensified HEX reactor involving an exothermic reaction of sodium thiosulfate oxidation by hydrogen peroxide is considered:

$$
2Na_2S_2O_3 + 4H_2O_2 \rightarrow Na_2S_3O_6 + Na_2SO_4 + 4H_2O
$$

Taking into account the above considerations, one can define state variables of the interconnected HEX reactor model as follows:

$$
x = \left(\begin{array}{c} x^1 \\ \vdots \\ x^i \\ \vdots \\ x^7 \end{array}\right) \quad with \quad x^i = \left(\begin{array}{c} T^i_p \\ T^i_p \\ T^i_w \\ C^i_1 \\ C^i_2 \end{array}\right)
$$

where x^i for $i = 1, ..., 7$ denotes the state vector of the i^{th} subsystem, T and C respectively represent the temperature and the concentration of the reactant, the subscripts p, u , and w respectively denote the process fluid, the utility fluid, and the plate wall and the subscripts 1 and 2 indicate the reactant $Na₂S₂O₃$ and $H₂O₂$ respectively. The mathematical model of the HEX reactor unit i is then given by

$$
\begin{cases}\n\dot{T}_p^i = \frac{F_p}{V_p^i} (T_p^{i-1} - T_p^i) + \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} (T_w^i - T_p^i) + Q_r^i \\
\dot{T}_u^i = \frac{F_u}{V_u^i} (T_u^{i-1} - T_u^i) + \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} (T_w^i - T_u^i) \\
\dot{T}_w^i = \frac{h_p A_p^i}{\rho_w V_w^i C_{p,w}} (T_p^i - T_w^i) + \frac{h_u A_u^i}{\rho_w V_w^i C_{p,w}} (T_u^i - T_w^i) \\
\dot{C}_1^i = \frac{F_p}{V_p^i} (C_1^{i-1} - C_1^i) - 2r^i \\
\dot{C}_2^i = \frac{F_p}{V_p^i} (C_2^{i-1} - C_2^i) - 4r^i\n\end{cases}
$$
\n(1)

where $F_p = F_{p,1} + F_{p,2}$ is the flow-rate of the process fluid, F_u is the flow-rate of the utility fluid. V, A, ρ , and C_p represent constant parameters signifying the volume, the heat exchange area, the density, and the specific heat of the material, respectively. Additionally, h_p and h_u denote the heat transfer coefficients corresponding to the process fluid and utility fluid with

$$
\begin{cases} h_p = \alpha_1 F_p + \alpha_2 \\ h_u = \beta_1 F_u + \beta_2 \end{cases}
$$
 (2)

where α_1 , α_2 , β_1 and β_2 are scalar factors that are experimentally determined. T_p^0 and T_u^0 are the inlet fluid temperatures of the process channel $(T_{p,in})$ and utility channel $(T_{u,in})$, while C_1^0 and C_2^0 are the inlet concentrations of $Na_2S_2O_3$ ($C_{1,in}$) and H_2O_2 ($C_{2,in}$), respectively. r denotes the speed of the reaction with

$$
r^i = k^i C_1^i C_2^i \tag{3}
$$

 k is the kinetic constant of the reaction governed by Arrhenius law

$$
k^i = k^0 \exp\left(-\frac{E^a}{RT_p^i}\right) \tag{4}
$$

where k^0 is the pre-exponential factor, E^a is activation energy, and R is the perfect gas constant. Q_r is the generated reaction heat with

$$
Q_r^i = -\frac{\Delta H_r r^i}{\rho_p C_{p,p}}\tag{5}
$$

where ΔH_r is the heat of the reaction.

The volumes and heat exchange areas of each reactor unit vary according to the relative length L_k corresponding to the thermocouple location as shown in Table I. The physical parameters of the HEX reactor are given in Table II and the parameters of the reaction are given in Table III.

TABLE I: Relative length of each unit of the simplified HEX reactor model

| Unit 1 | \parallel Unit 2 \parallel Unit 3 | | \vert Unit 4 \vert Unit 5 \vert Unit 6 | Unit |
|---|---------------------------------------|--|--|------|
| L_k 0.022 0.02 0.059 0.039 0.176 0.342 0.342 | | | | |

TABLE II: Physical parameters of the simplified HEX reactor model [13]

| Parameter | Value | Unit |
|--------------------|----------------------------------|--|
| V_p | 2.68×10^{-5} | m ³ |
| V_u | 1.141×10^{-4} | $\rm m^3$ |
| V_{w} | 2.7×10^{-3} | m ³ |
| A_p | $5.\overline{36 \times 10^{-2}}$ | m ² |
| A_u | 2.282×10 | m ² |
| $C_{p,p}, C_{p,u}$ | 4.186×10^{3} | $J \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ |
| $C_{p,w}$ | 5×10^2 | $J \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ |
| ρ_p, ρ_u | 10^{3} | $\text{kg} \cdot \text{m}^{-3}$ |
| ρ_w | 8×10^3 | $kg \cdot m^{-3}$ |
| α_1 | 2.0787×10^{9} | $\rm W\cdot m^{-2}\cdot K^{-1}$ |
| α_2 | $2.\overline{7323 \times 10^3}$ | $\overline{W \cdot m^{-2} \cdot K^{-1}}$ |
| β_1 | 1.5055×10^8 | $\overline{W \cdot m^{-2} \cdot K^{-1}}$ |
| β_2 | 2.5133×10^{3} | $\overline{W \cdot m^{-2} \cdot K^{-1}}$ |

TABLE III: Parameters of the reaction [13]

B. Observer design model

However, the number of thermocouples that could be installed inside the process plate is quite limited and the reactant concentrations cannot be measured. There is hence a lack of temperature measurements and the heat generated by the chemical reactions cannot be determined in real time. In the following, one will show that this relevant information from a safe operation point of view can be estimated using a suitable observer. To this end, Let us first p oint o ut that none of the temperatures of the plate wall is measurable and that the available temperatures for the process plate (resp.

the utility plate) are the inlet process fluid temperature $T_{p,in}$ and the output process temperatures of each unit $\left\{T_p^i\right\}_{i\in[1,7]}$ (resp. the inlet utility fluid temperature $T_{u,in}$ and the output temperature of the last cell $y_u = T_u^7$). Indeed, it is possible to design high gain observers for each reactor unit to estimate the unmeasurable temperatures $\{T_u^i\}_{i \in [1,6]}$ and $\{T_w^i\}_{i \in [1,7]}$ together the generated reaction heat $\{Q_r^i\}_{i \in [1,7]}$ using the accessible output of each unit

$$
\begin{cases}\ny^i = T_p^i \quad \text{for } i = 1, \dots, 6 \\
y^7 = \left(\begin{array}{c}\nT_p^7 \\
T_u^7\n\end{array}\right)\n\end{cases} \tag{6}
$$

Bearing in mind the high gain observer design culture, a suitable observer design model for the intensified HEX reactor can be elaborated from two sub-models. The first one is given by the model of the first six reactor units which outputs are the process temperatures ${T_p^i}_{i \in [1,6]}$ and may be written as follows

$$
\begin{cases}\n\dot{T}^i_u = \frac{F_u}{V_u^i} (T_u^{i-1} - T_u^i) + \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} (T_w^i - T_u^i) \\
\dot{T}^i_w = \frac{h_p A_p^i}{\rho_w V_u^i C_{p,w}} (T_p^i - T_w^i) + \frac{h_u A_u^i}{\rho_w V_u^i C_{p,w}} (T_u^i - T_w^i) \\
\dot{T}^i_p = \frac{F_p}{V_p^i} (T_p^{i-1} - T_p^i) + \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} (T_w^i - T_p^i) + Q_r^i \\
\dot{Q}_r^i = \epsilon^i\n\end{cases} \tag{7}
$$

where ϵ is an unknown bounded function. One can easily derive a state space representation of this model around the state vector and the output

$$
x = \begin{pmatrix} x^1 \\ \vdots \\ x^i \\ \vdots \\ x^6 \end{pmatrix} \text{ with } x^i = \begin{pmatrix} x^{i,1} \\ x^{i,2} \end{pmatrix} \text{ and } y = \begin{pmatrix} y^1 \\ \vdots \\ y^i \\ \vdots \\ y^6 \end{pmatrix}
$$

where

$$
x^{i,1} = \begin{pmatrix} T_u^i \\ T_w^i \end{pmatrix}, \quad x^{i,2} = \begin{pmatrix} T_p^i \\ Q_r^i \end{pmatrix} \quad and \quad y^i = T_p^i
$$

The second one is given by the $7th$ reactor unit whose output is composed by the process fluid temperature T_p^7 together with the utility fluid temperature T_u^7 and can be rewritten under the following form with $i = 7$.

$$
\begin{cases}\n\dot{T}_p^i = \frac{F_p}{V_p^i} (T_p^{i-1} - T_p^i) + \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} (T_w^i - T_p^i) + Q_r^i \\
\dot{T}_u^i = \frac{F_u}{V_u^7} (T_u^{i-1} - T_u^i) + \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} (T_w^i - T_u^i) \\
\dot{Q}_r^i = \epsilon^i \\
\dot{T}_w^i = \frac{h_p A_p^i}{\rho_w V_w^i C_{p,w}} (T_p^i - T_w^i) + \frac{h_u A_u^i}{\rho_w V_w^i C_{p,w}} (T_u^i - T_w^i)\n\end{cases} \tag{8}
$$

One can easily derive a state space representation of this model around the state vector x^i and the output y^i respectively given by

$$
x^i = \left(\begin{array}{c} x^{i,1} \\ x^{i,2} \end{array}\right)
$$

with

$$
x^{i,1} = \left(\begin{array}{c} T_p^i \\ T_u^i \end{array}\right), \quad x^{i,2} = \left(\begin{array}{c} Q_r^i \\ T_w^i \end{array}\right) \quad and \quad y^i = x^{i,1}
$$

The HEX reactor has been modularly modeled based on its available outputs by the sub-models (7) and (8) that can be rewritten under state space representation. The latter will be used to design a SHGCO in the next section.

III. THE SHGCO DESIGN

The intensified HEX reactor cascade model (7)-(8) has been developed by properly using the variability of the available output measurements. The related state representation can be naturally used to design a SHGCO to deal with the challenging estimation problem of the intensified HEX reactor, namely an admissible estimation of the involved temperature and reaction heat distribution according to the adopted cascade decomposition of the reactor. This SHGCO is derived from a genuine compilation of the available results on the high gain observer design (See [7] and reference list therein). Of particular interest, the proposed SHGCO incorporates an appropriate saturation function to deal with the ubiquitous peaking phenomenon of the high gain principle. The SHGCO will be gradually presented according to the available output measurements using the intensified HEX reactor cascade model $(7)-(8)$.

A. SHGCO design for the subsystems with one output signal

For the first six reactor units model (7) , the involved estimation problem is performed using two observers according to the underlying model state decomposition. More specifically, the utility fluid and plate wall temperatures, namely the state variables involved in the sub-state

$$
x^{i,1} = \left(\begin{array}{c} T_u^i \\ T_w^i \end{array}\right) \quad \text{for } i \in [1,6]
$$

and first estimated using the following observer family.

$$
\dot{\hat{x}}^{i,1} = F_{i,1}\hat{x}^{i,1} + G_{i,1}(\hat{x}^{i,1}, u) \quad \text{for } i \in [1, 6] \tag{9}
$$

with

$$
F_{i,1} = \begin{pmatrix} -\frac{F_u}{V_u^i} - \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} & \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} \\ \frac{h_u A_u^i}{\rho_w V_u^i C_{p,w}} & -\frac{h_p A_p^i}{\rho_w V_u^i C_{p,w}} - \frac{h_u A_u^i}{\rho_w V_u^i C_{p,w}} \end{pmatrix}
$$

$$
G_{i,1}(\hat{x}^{i,1}, u) = \begin{pmatrix} \frac{F_u}{V_u^i} \hat{T}_u^{i-1} \\ \frac{h_p A_p^i}{\rho_w V_u^i C_{p,w}} T_p^i \end{pmatrix}
$$

where $\hat{T}^0_n = T_{u,in}$ is the inlet temperature of the utility fluid. These temperatures will be employed in the subsequent process fluid temperature estimation.

And the process fluid temperatures and reaction heat, namely the state variables involved in the sub-state

$$
x^{i,2} = \left(\begin{array}{c} T_p^i \\ Q_r^i \end{array}\right) \quad \text{for } i \in [1,6]
$$

and subsequently estimated using the following observer family together with the above temperature estimation process

$$
\begin{cases}\n\dot{\hat{T}}_p^i = \frac{F_p}{V_p^i} (\hat{T}_p^{i-1} - \hat{T}_p^i) + \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} (\hat{T}_w^i - \hat{T}_p^i) + \hat{Q}_r^i - \theta H_1^i \\
\dot{\hat{Q}}_r^i = -\theta H_2^i\n\end{cases}
$$
\n(10)

with

$$
\begin{cases}\nH_1^i = k_1^i e_{T_p^i} \\
H_2^i = s a t_\nu \left(\theta \frac{k_2^i}{k_1^i} H_1^i\right)\n\end{cases} \tag{11}
$$

$$
sat_r(z) = \begin{cases} z, & \text{if } |z| \le r \\ r \ sign(z), & \text{if } |z| > r \end{cases} \quad \forall z \in \mathbb{R} \tag{12}
$$

where $T_p^0 = T_{p,in}$ is the inlet temperature of the process fluid. $e_{T_n^i} = \hat{T}_p^i - T_p^i$ denotes the estimation error, $sign(\cdot)$ is the signum function, $\theta > 0$ is the high gain design parameter and k_1^i , k_2^i , r and ν denotes the design parameters involved in the observer gain and the saturation function to recover the observer strong stability and convergence requirements that are comprehensively presented in [7].

B. SHGCO Design for the subsystem with two output elements

Different from the first six units, the seventh reactor unit model (8) has an additional output measurement, namely the utility fluid temperature T_u^7 . The involved temperature and reaction heat estimation can be performed by the following suitable high gain observer with $i = 7$.

$$
\begin{cases}\n\dot{\hat{x}}^{1,i} = F_i \hat{x}^{2,i} + G_i(\hat{x}^{1,i}, u) - \theta H_1^i \\
\dot{\hat{x}}^{2,i} = \bar{\epsilon}^i - \theta F_i^{-1} H_2^i\n\end{cases}
$$
\n(13)

with

$$
\hat{x}^{i,1} = \begin{pmatrix} \hat{T}_p^i \\ \hat{T}_u^i \end{pmatrix} \quad and \quad \hat{x}^{i,2} = \begin{pmatrix} \hat{Q}_r^i \\ \hat{T}_w^i \end{pmatrix}
$$
\n
$$
F_i = \begin{pmatrix} 1 & \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} \\ 0 & \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} \end{pmatrix}
$$
\n
$$
G_i(\hat{x}^{i,1}, u) = \begin{pmatrix} \frac{F_p}{V_p^i} (T_p^{i-1} - \hat{T}_p^i) - \frac{h_p A_p^i}{\rho_p V_p^i C_{p,p}} \hat{T}_p^i \\ \frac{F_u}{V_u^i} (\hat{T}_u^{i-1} - \hat{T}_u^i) - \frac{h_u A_u^i}{\rho_u V_u^i C_{p,u}} \hat{T}_u^i \end{pmatrix}
$$
\n
$$
\bar{\epsilon}^i = \begin{pmatrix} 0 \\ \frac{h_p A_p^i}{\rho_w V_u^i C_{p,w}} (T_p^i - \hat{T}_w^i) + \frac{h_u A_u^i}{\rho_w V_w^i C_{p,w}} (\hat{T}_u^i - \hat{T}_w^i) \\ \frac{h_i^i}{\rho_v V_u^i C_{p,w}} \end{pmatrix}
$$
\n
$$
H_1^i = \begin{pmatrix} k_1^i e_{T_p^i} \\ k_1^i e_{T_u^i} \end{pmatrix} \quad and \quad H_2^i = \begin{pmatrix} sat_{\nu_1} \left(\theta \frac{k_2^i}{k_1^i} H_{1,1}^i \right) \\ sat_{\nu_2} \left(\theta \frac{k_2^i}{k_1^i} H_{1,2}^i \right) \end{pmatrix}
$$

where $e_{T_n^i} = \hat{T}_p^i - T_p^i$, $e_{T_n^i} = \hat{T}_u^i - T_u^i$ denote the temperature estimation error and the various design parameters are specified according to the observer strong stability and convergence requirements that are comprehensively presented in $\lceil 7 \rceil$.

IV. SIMULATION RESULTS

The effectiveness of the SHGCO has been illustrated in a simulation framework involving the physical model of the intensified HEX reactor presented in under the experimental planning proposed in [1] for real experiment consistency purposes. Reactants are introduced into the process channel with the identical temperature $T_{p,in} = 21 \degree \text{C}$ and with different flow rates to achieve the optimal reaction rate: $F_{p,1}$ = 1.3056 × 10⁻⁶ m³⋅s⁻¹, $F_{p,2}$ = 6.3889 × 10⁻⁷ $m^3 s^{-1}$. The concentrations are both set to 9% in mass. Water is injected into the utility channel with a higher temperature $T_{u,in} = 59.4$ °C and a faster flow-rate $F_u =$ 3.125×10^{-5} m³⋅s⁻¹. Initial temperatures of each subsystem are the same: $T_p^i(0) = T_{p,in}$, $T_u^i(0) = T_{u,in}$, $T_w^i(0) = 25$ ◦C. The SHGCO shares the same initial temperatures, but these values differ from those of the system to illustrate the observer convergence. $\hat{T}_p^i(0) = 90\% \ T_p^i(0), \ \hat{T}_u^i(0) =$ $90\% \ T_u^i(0), \hat{T}_w^i(0) = 90\% \ T_u^i(0).$

The temperature state estimates are depicted in Figure 3. In the figure, the solid lines represent temperatures acquired from the simulated system, while the dashed lines represent temperatures estimated using the designed SHGCOs. It is obvious that all the temperatures of each reactor unit are well estimated after the transition period. Despite the distinct construction of SHGCOs associated with the 7th unit and the combined observers related to the rest units, the temperature estimates exhibit excellent accuracy and a satisfactory speed of convergence because of the comprehensive utilization of available measurements.

The estimates of the generated reaction heat Q_r are given in Figure 4 where they are compared to their true values issued from the simulated model (1) by considering the expression given by (5) for the reaction heat. Due to varying reactant concentrations among different units, the heat generated by each unit differs as well. Nevertheless, the estimation of the reaction heat is well performed. It is worth noticing that the peak phenomenon has been eliminated for both state estimation and parameter estimation due to the implementation of the saturation function.

V. CONCLUSION

The ultimate motivation for this paper was to provide a suitable framework for the safe operation of intensified HEX reactors using the available high gain observer culture. An engineering approach has been adopted to deal with the observer design bearing in mind the essential modelling and implementation requirements. The essential design and implementation features have been comprehensively presented, namely the observer model design and the SHGCO, under the benediction of the recent available fundamental potential on the high gain observer system engineering. Two design features are worth to be pointed out. Firstly, the cascade modeling is properly used to elaborate an adequate model of the intensified H EX r eactor, p roviding t hereby a n accurate distribution of the temperature inside the reactor. Secondly, the high gain observer design framework is appropriately

(a) Estimation of process fluid temperature: T_p and \tilde{T}_p

(b) Estimation of utility fluid temperature: T_u and \hat{T}_u

(c) Estimation of plate wall temperature: T_w and T_w

Fig. 3: Temperature state estimation of the HEX reactor

Fig. 4: Parameter estimation of the reaction heat: Q_r and \hat{Q}_r

used to provide an admissible estimation of the temperatures and reaction heat inside the reactor using the available temperature measures. Of particular interest, an adequate saturation function has been used to deal with the ubiquitous peaking phenomenon of the high gain principle. The effectiveness of the proposed SHGCO has been illustrated by probing simulation results.

The designed SHGCO facilitates the acquisition of unmeasurable temperatures and reaction heat, enabling the monitoring of internal states and parameters within the HEX reactor system. Building upon this capability, the subsequent step involves the development of observer-based fault diagnosis algorithms and fault-tolerant control methods to ensure the secure operation of the HEX reactor.

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REFERENCES

- [1] Z. Anxionnaz, M. Cabassud, C. Gourdon, P. Tochon, Heat exchanger/reactors (HEX reactors): concepts, technologies: state-of-theart[J]. Chemical Engineering and Processing: Process Intensification, 2008, 47(12): 2029-2050.
- [2] M. Cabassud, C. Gourdon. Intensification of heat transfer in chemical reactors: heat exchanger reactors[J]. Novel Concepts in Catalysis and Chemical Reactors: Improving the Efficiency for the Future, 2010: 261-287.
- [3] F. Théron, Z. Anxionnaz-Minvielle, M. Cabassud, C. Gourdon, P. Tochon. Characterization of the performances of an innovative heatexchanger/reactor[J]. Chemical Engineering and Processing: Process Intensification, 2014, 82: 30-41.
- [4] J. P. Gauthier, H. Hammouri, S. Othman, A simple observer for nonlinear systems applications to bioreactors[J]. IEEE Transactions on automatic control, 1992, 37(6): 875-880.
- [5] J. P. Gauthier, I. Kupka, Deterministic observation theory and applications[M]. Cambridge university press, 2001.
- [6] H. K. Khalil, L. Praly, High-gain observers in nonlinear feedback control[J]. International Journal of Robust and Nonlinear Control, 2014, 24(6): 993-1015.
- [7] M. Farza, A. Ragoubi, S. Hadj Said, M. M'saad, Improved high gain observer design for a class of disturbed nonlinear systems[J]. Nonlinear Dynamics, 2021, 106: 631-655.
- [8] M. Zhang, B. Dahhou, M. Cabassud, Z. Li, Actuator fault detection and isolation via input reconstruction: application to intensified heat exchanger reactor[C]//2015 23rd Mediterranean Conference on Control and Automation (MED). IEEE, 2015: 322-327.
- [9] M. Zhang, B. Dahhou, M. Cabassud, Z. Li, Faults isolation in intensified continuous HEX reactor with parameter uncertainties[C]//The 26th International Workshop on Principles of Diagnosis (DX-2015). 2015.
- [10] M. Zhang, Z. Li, M. Cabassud, B. Dahhou, An integrated FDD approach for an intensified HEX/Reactor[J]. Journal of Control Science and Engineering, 2018, 2018: 1-16.
- [11] X. Han, Z. Li, M. Cabassud, B. Dahhou, A Comparison Study of Nonlinear State Observer Design: Application to an Intensified Heat-Exchanger/Reactor[C]//2020 28th Mediterranean Conference on Control and Automation (MED). IEEE, 2020: 162-167.
- [12] X. Han, R. Rammal, M. He, Z. Li, M. Cabassud, B. Dahhou, Dynamic and sensor fault tolerant control for an intensified heatexchanger/reactor[J]. European Journal of Control, 2023, 69: 100736.
- [13] M. He, Z. Li, X. Han, M. Cabassud, B. Dahhou, Development of a Numerical Model for a Compact Intensified Heat-Exchanger/Reactor[J]. Processes, 2019, 7(7): 454.
- [14] M. Farza, M. M'Saad, L. Rossignol, Observer design for a class of MIMO nonlinear systems[J]. Automatica, 2004, 40(1): 135-143.
- [15] H. Hammouri, G. Bornard, K. Busawon, High gain observer for structured multi-output nonlinear systems[J]. IEEE Transactions on automatic control, 2010, 55(4): 987-992.
- [16] H. K. Khalil, Cascade high-gain observers in output feedback control[J]. Automatica, 2017, 80: 110-118.
- [17] M. Farza, O. Hernández-González, T. Ménard, B. Targui, M. M'Saad, C. M. Astorga-Zaragoza, Cascade observer design for a class of uncertain nonlinear systems with delayed outputs[J]. Automatica, 2018, 89: 125-134.
- X. Han, M. He, N. D. M. Raimondi, M. Cabassud, B. Dahhou, $[18]$ Distributed adaptive observer-based Fault Diagnosis for an Intensified Heat Exchanger/Reactor[C]//2023 31st Mediterranean Conference on Control and Automation (MED). IEEE, 2023: 37-42.