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Review Article

Robust Control for Uncertain Semi-batch Free-radical Polymerization Reactor

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Abstract
In this work, a robust control scheme is formulated for uncertain semi-batch free radical polymerization reactor that produces polyacrylamide. Adaptive fractional order sliding mode controllers (AFSMC) are developed to drive the average molecular weight and the monomer concentration to follow the reference trajectories. Moreover, the gains of the reaching laws are updated online. As a result, the requirement of the information of the uncertainties' bounds are relaxed. The closed loop stability of the system has been guaranteed using the Lyapunov function. Comparison of simulation results are provided to show the fruitfulness of the proposed method.

Keywords: Fractional order, sliding mode control, adaptive control, semi-batch reactor.

I. INTRODUCTION
Chemical reactors constitute the building block of every chemical industry, and in the present competitive framework, managing various operating variables and meeting product requirements is of paramount importance [1], [2]. Batch and semi-batch operations are preferred for high-value low volume chemicals such as fine chemicals, pharmaceuticals and polymers, since the reactors can be used for various products [3]. In recent years, techniques for state estimation [4], [5], [6], [7] and control methods have advanced to address industrial problems in chemical reactors and unit operations. Advanced manufacturing techniques are important because they allow the efficient use of feedstock materials, energy, and labor while also improving safety in a chemical plant. The combination of mechanistic model complexity and inadequate real-time characterization techniques poses crucial challenges, particularly in the polymer industry.

There are generally different types of uncertainties affecting the batch processes; The uncertainties can be largely classified into three types: external disturbances, noises and parameter variations [8], [9]. External disturbances include concentration of reactants, temperature, purity of reactants and degree of mixing. Parameter variations comprise discrepancies in mass / heat transfer coefficients, kinetic parameters, etc. noises come from sensing devices. The effects of the uncertainties have been thoroughly investigated by the control community.

In [10], an economic model predictive controller (EMPC) has been designed to keep the states of the batch reactors within certain constraints. In [11], a multi-stage EMPC has been developed using an unscented Kalman filter. However, in the presence of parametric uncertainties, the performances of the EMPC can be hampered. A robust nonlinear model predictive control (NMPC) has been designed for an uncertain batch reactor [8]. In [12], a robust NMPC has been implemented for a chemical reactor and its performances were validated via experiment. In [13], a robust control strategy is formulated to regulate the temperature of a batch reactor. In [14], a nonlinear proportional-integral control method is proposed to improve the trajectory tracking accuracy of a batch reactor. In [15], a robust model predictive controller is implemented for a batch reactor to mitigate fault and enhance the performance of the process. In [16], a robust model predictive control is developed for a multi-phase batch polymerization reactor to counter time delay, dynamic uncertainties, and disturbances. In [17], a nonlinear model predictive controller is developed to prevent thermal runaway in a batch reactor. In [18], a robust SMC has been designed for semi batch polymerization reactor in the presence of

parameter variations. A robust SMC with SM observer was suggested in [19] for temperature tracking control of the batch reactor. In [20], a deadbeat control approach is employed to achieve the optimal temperature performance of a batch reactor. In [21], an input-output SMC has been designed for a batch process with uncertainties.

In [22], an adaptive temperature controller combined with an extended Kalman filter is constructed for a semi-batch polymerization reactor with unknown kinetic parameters. In [23], a predictive controller with a probabilistic least squares algorithm with a forgetting factor is designed for a batch system. In [24], a neuro-adaptive generic model control of batch reactors has been investigated. In [25], a neuro-adaptive cascade control of batch reactor temperature was studied. In [26], adaptive control of batch reactor with unknown heat transfer coefficients was presented. An adaptive backstepping control method has been applied to a polymerization reactor with uncertainties of parameters. In [27], an adaptive model predictive control has been proposed to rethegulate the average molecular weight of a polymer in a polymerization reactor. In [28], an adaptive input-output feedback linearization controller with a sigma-point Kalman filter has been implemented for a batch reactor.

In this article, we proposed a robust AFSMC for semi batch polymerization reactor to achieve the target average molecular weight and monomer concentration. The knowledge of the upper bounds of the uncertainties is not required. We employed adaptation laws to estimate the upper bounds online.

The structure of the paper is as follows: The mathematical model of the semi-batch reactor is presented in Section II. The AFSMC and the PI controllers are developed in Section III. The simulation results are given in Section IV. We conclude the work in Section V.

II. MATHEMATICAL MODEL

The underlying dynamic model describes the free-radical polymerization of acrylamide using potassium persulfate (KPS) as initiator. The batch reactor model was built and experimentally validated by [29]. The dynamic equations are as follows

$$\frac{dN_m}{dt} = -(K_{fm} + K_p)r_0 N_m + F_m C_{mf} - F_0 C_m \quad (1)$$

$$\frac{dN_i}{dt} = -K_d N_i + F_i C_{if} - F_0 C_i \quad (2)$$

$$\frac{dN_s}{dt} = -K_{fs} N_s r_0 + F_i C_{sif} + F_m C_{smf} - F_0 C_s \quad (3)$$

$$\frac{d(\lambda_0 V)}{dt} = \left(K_{fm} N_m + K_{td} r_0 V + K_{fs} N_s\right)\gamma r_0 + \frac{1}{2} K_{tc} r_0^2 V - F_0 \lambda_0 \quad (4)$$

$$\frac{d(\lambda_1 V)}{dt} = \left[\left(K_{fm} N_m + K_{td} r_0 V + K_{fs} N_s\right)(2\gamma - \gamma^2) + K_{tc} r_0 V\right] \frac{r_0}{(1-\gamma)} - F_0 \lambda_1 \quad (5)$$

$$\frac{d(\lambda_2 V)}{dt} = \left[\left(K_{fm} N_m + K_{td} r_0 V + K_{fs} N_s\right)(\gamma^3 - 3\gamma^2 - 4\gamma) + K_{tc} r_0 V(\gamma + 2)\right] \frac{r_0}{(1-\gamma)^2} - F_0 \lambda_2 \quad (6)$$

Were

$$N_m = C_M V,\ N_i = C_i V, N_s = C_s V$$

$$\gamma = \frac{K_{pC_m}}{K_{fm} C_m + K_{fs} C_s + K_p C_m + K_{tc} r_0 + K_{td} r_0}$$

$$r_0 = \sqrt{\frac{2 C_i K_d}{K_{tc} + K_{td}}}$$

N_i, N_m, and N_s denote the number of moles of the initiator, monomer and solvents respectively, C_i, C_m, and C_s represent the concentration of the initiator, monomer and solvent respectively, λ_0, λ_1 and λ_2 represent the moments of dead polymer, V stand for the volume of internal contents of the reactor, $K_{fm}, K_{fs}, K_d, K_p K_{tc}$ and K_{td} are kinetic rate constants. The outputs taken from the system are as follows

$$C_m = \frac{N_m}{V} \tag{7}$$

$$M = w_m \frac{\lambda_2 V}{\lambda_1 V} \tag{8}$$

Were

$$V = \frac{w_s N_s}{\rho_s} + \frac{w_i N_i}{\rho_i} + \frac{w_m N_m}{\rho_m} + \frac{w_m \lambda_1 V}{\rho_p}$$
$$\rho_s = -0.00310T^2 - 0.14670T + 1003.0$$

Differentiating C_m with respect to time gives

$$\dot{C}_m = \frac{\dot{N}_m}{V} + \frac{N_m \dot{V}}{V^2} = A_1 + G_{11} F_m + G_{12} F_i \tag{9}$$

Were

$$A_1 = \frac{1}{V}\left(-\left(K_{fm} + K_p\right) r_0 N_m - F_0 C_m\right) + \frac{N_m w_m}{\rho_m V^2}\left(-\left(K_{fm} + K_p\right) r_0 N_m - F_0 C_m\right) + \frac{N_m w_s}{\rho_s V^2}\left(-K_{fs} N_s r_0 - F_0 C_s\right) + \frac{N_m w_i}{\rho_i V^2}\left(-K_d N_i - F_0 C_i\right) + \frac{w_m N_m}{V^2 \rho_p}\frac{d(\lambda_1 V)}{dt}$$

$$G_{11} = \frac{C_{mf}}{V} + \frac{N_m w_m C_{mf}}{\rho_m V^2} + \frac{N_m w_i C_{smf}}{\rho_i V^2}$$

$$G_{12} = \frac{N_m w_s C_{sif}}{\rho_s V^2} + \frac{N_m w_i C_{if}}{\rho_i V^2}$$

Differentiating M with respect to time yields

$$\dot{M} = -w_m \frac{\lambda_2 V}{(\lambda_1 V)^2}\frac{d(\lambda_1 V)}{dt} + w_m \frac{1}{\lambda_1 V}\frac{d(\lambda_2 V)}{dt} \tag{10}$$

The second time-derivative of M gives

$$\ddot{M} = \frac{\partial \dot{M}}{\partial N_m}\dot{N}_m + \frac{\partial \dot{M}}{\partial N_i}\dot{N}_i + \frac{\partial \dot{M}}{\partial N_s}\dot{N}_s + \frac{\partial \dot{M}}{\partial (\lambda_1 V)}\frac{d(\lambda_1 V)}{dt} \tag{11}$$

Were

$$A_2 = \frac{\partial \dot{M}}{\partial N_m}\left(-\left(K_{fm} + K_p\right) r_0 N_m - F_0 C_m\right) - \frac{\partial \dot{M}}{\partial N_i}\left(K_d N_i + F_0 C_i\right) - \frac{\partial \dot{M}}{\partial N_s}\left(K_{fs} N_s r_0 + F_0 C_s\right) + \frac{\partial \dot{M}}{\partial (\lambda_1 V)}\frac{d(\lambda_1 V)}{dt} + \frac{\partial \dot{M}}{\partial (\lambda_2 V)}\frac{d(\lambda_2 V)}{dt}$$

$$G_{21} = \frac{\partial \dot{M}}{\partial N_m}\left(C_{mf}\right) + \frac{\partial \dot{M}}{\partial N_s}\left(C_{smf}\right)$$

$$G_{22} = \frac{\partial \dot{M}}{\partial N_i}\left(C_{if}\right) + \frac{\partial \dot{M}}{\partial N_s}\left(C_{sif}\right)$$

III. ADAPTIVE FRACTIONAL ORDER SLIDING MODE CONTROL

In this section, we proposed AFSMC to control C_m and M and show excellent robustness for external disturbances and parameter variations. The Caputo definition of fractional order derivatives is given by [30], [31]:

$$D_t^{\alpha} f(t) = \frac{1}{\Gamma(\eta - \alpha)} \int_0^t \frac{f^{\eta}(\tau)}{(t-\tau)^{\alpha - \eta + 1}} d\tau \tag{12}$$

Where η is an integer such that $\eta - 1 < \alpha < \eta$ and $\Gamma(.)$ is a Gamma function. Define the error between C_m and C_{md} as $z_c = C_m - C_{md}$. Then, the fractional order SMC surface can be expressed as

$$S_c = z_c + \lambda_c \int_{t_0}^{t} z_c dt + \Lambda_c D^{\alpha-1} z_c \tag{13}$$

Where λ_c and Λ_c are positive constants. The time derivative of S_c is computed as

$$\dot{S}_c = \dot{z}_c + \lambda_c z_c + \Lambda_c D^{\alpha} z_c \tag{14}$$

Define the tracking error between M and M_d as $z_m = M - M_d$. Then, the fractional order SMC surface is given by

$$S_M = \dot{z}_M + \lambda_M \int_{t_0}^{t} z_M dt + \Lambda_M D^{\alpha-1} z_M \tag{15}$$

Where λ_M and Λ_M are positive constants. The time derivative of S_c is computed as

$$\dot{S}_M = \ddot{z}_M + \lambda_c z_M + \Lambda_M D^{\alpha} z_M \tag{16}$$

Let

$$S = [S_c S_M]^T, A = [A_1 \quad A_2]^T, U = [F_M F_i]^T,$$
$$V = \begin{bmatrix} -\dot{C}_{md} + \lambda_c z_c + \Lambda_c D^{\alpha} z_c \\ -\ddot{M}_d + \lambda_M z_M + \Lambda_M D^{\alpha} z_M \end{bmatrix}, G = \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}$$

Equations (14) and (16) can be written in matrix form as follows

$$\dot{S} = A + GU + V \tag{17}$$

The equivalent control law can be obtained when $S = \dot{S} = 0$ as

$$U_{eq} = G^{-1}[-A - V] \tag{18}$$

The adaptive reaching law is designed as

$$U_r = -G^{-1}\left[\hat{K}|S|\,\mathrm{sgn}(S)\right] \tag{19}$$

Where the diagonal matrix $\hat{K}$ is the estimate of the diagonal matrix K, $|S|\mathrm{sgn}(S) = [|S_c|\mathrm{sgn}(S_c)|S_M|\mathrm{sgn}(S_M)]^T$. The total control law is expressed as

$$U = U_{eq} + U_r = -G^{-1}\left[A + V + \hat{K} \parallel S \parallel \mathrm{sign}(S)\right] \tag{20}$$

Since $\det(G) = G_{11}G_{22} - G_{12}G_{21} \neq 0, G^{-1}$ exist. The adaptive law is designed as

$$\dot{\hat{K}} = \beta |S|^2 \tag{21}$$

Where $\beta > 0$ is a diagonal matrix, $|S|^2 = [|S_c|^2|S_M|^2]^T$ Theorem 1: For the semi-batch reactor system (1)-(6), under the FSM manifolds (13) and (15), and the adaptive controller (20), the tracking errors and the sliding variables will converge to zero

Proof 1: Consider the Lyapunov function

$$L = \frac{1}{2} S^T S + \frac{1}{2} \tilde{2} K^T \beta^{-1} \tilde{K} \tag{22}$$

By differentiating L, we get

$$\dot{L} = S^T \dot{S} + \tilde{K}^T \beta^{-1} \dot{\tilde{K}} \tag{23}$$

Inserting (20) into (23) gives

$$\begin{aligned} \dot{L} &= S^T[-\hat{K}|S|\mathrm{sign}(S)] - \tilde{K}^T \beta^{-1} \dot{\hat{K}} \\ &= S^T[-(K - \tilde{K})|S|\mathrm{sign}(S)] - \tilde{K}^T \beta^{-1} \dot{\hat{K}} \end{aligned} \tag{24}$$

Substituting the adaptation law (21) into (24), one has

$$\dot{L} \leq -K|S|^2 < 0 \tag{25}$$

A. FEEDBACK LINEARIZATION CONTROLLER (FC)

The performance of the proposed AFSCM is compared with that of FC. Equations (9) and (11) can be written in matrix form as

$$\begin{bmatrix} \dot{C}_m \\ \ddot{M} \end{bmatrix} = A + GU \tag{26}$$

The linearizing controller is thus

$$U = G^{-1}[-A + P] \tag{27}$$

Where P is an auxiliary input designed as

$$P = \begin{bmatrix} R_{pc}z_c + R_{ic}\int_{t_0}^{t} z_c dt \\ R_{pM}z_M + R_{iM}\int_{t_0}^{t} z_M dt \end{bmatrix} \tag{28}$$

Where R_{pc}, R_{ic}, R_{pM} and R_{iM} are positive parameters.

IV. RESULTS

A comparison between the AFSMC scheme and the FC method is provided to illustrates the benefits of proposed method in this section. The parameters of the semi-batch polymerization reactor are adopted from [29]. The parameters of the AFSMC are as follows: $\lambda_c = 8, \Lambda_c 4, \lambda_c = 12, \Lambda_c = 10, \beta_c = 5, \beta_M = 3$, the fractional order derivative is $\alpha = 0.4$. The parameters of the FC are as follows: $R_{pc} = 5, R_{ic} = 4, R_{iM} = 8, R_{pM} = 8$.

Figs. 1-4 depict the simulation results. As shown in Fig. 1, under the action of AFSMC, the outputs have lower rise time, no overshoot and settle faster. The poor performances of FC are due to the lack of robustness against uncertainties. The tracking errors converge to zero quicker under the action of AFSMC as presented in Fig. 2. The control inputs are presented in 3. The estimated upper bounds of the uncertainties are shown in Fig. 4.

V. CONCLUSIONS

The AFSMC technique has been developed for the uncertain semi-batch polymerization reactor. The upper bounds of the uncertainties are estimated by adaptive laws. The proposed scheme can also guarantee that the tracking errors variables converge to the origin. Simulation results depict the efficacy of the proposed method.

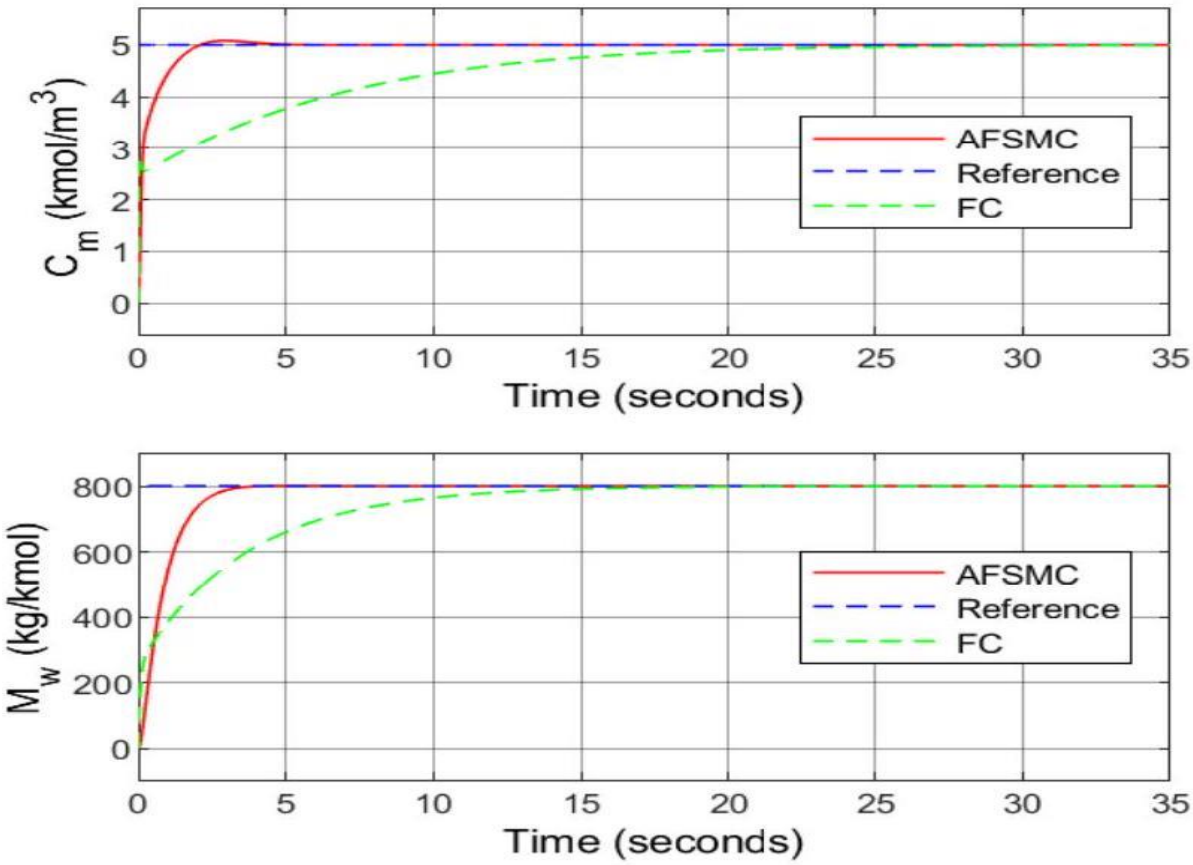

FIGURE 1: The outputs' responses

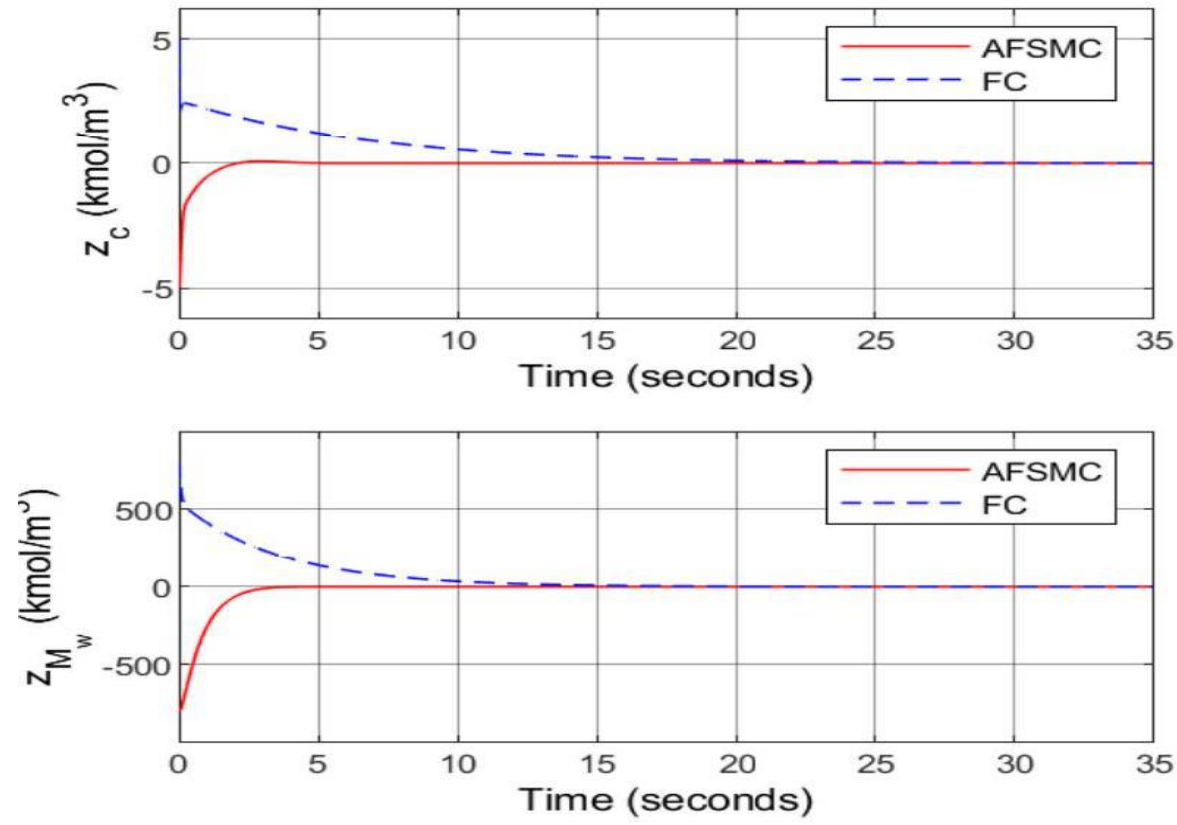

FIGURE 2: The tracking errors

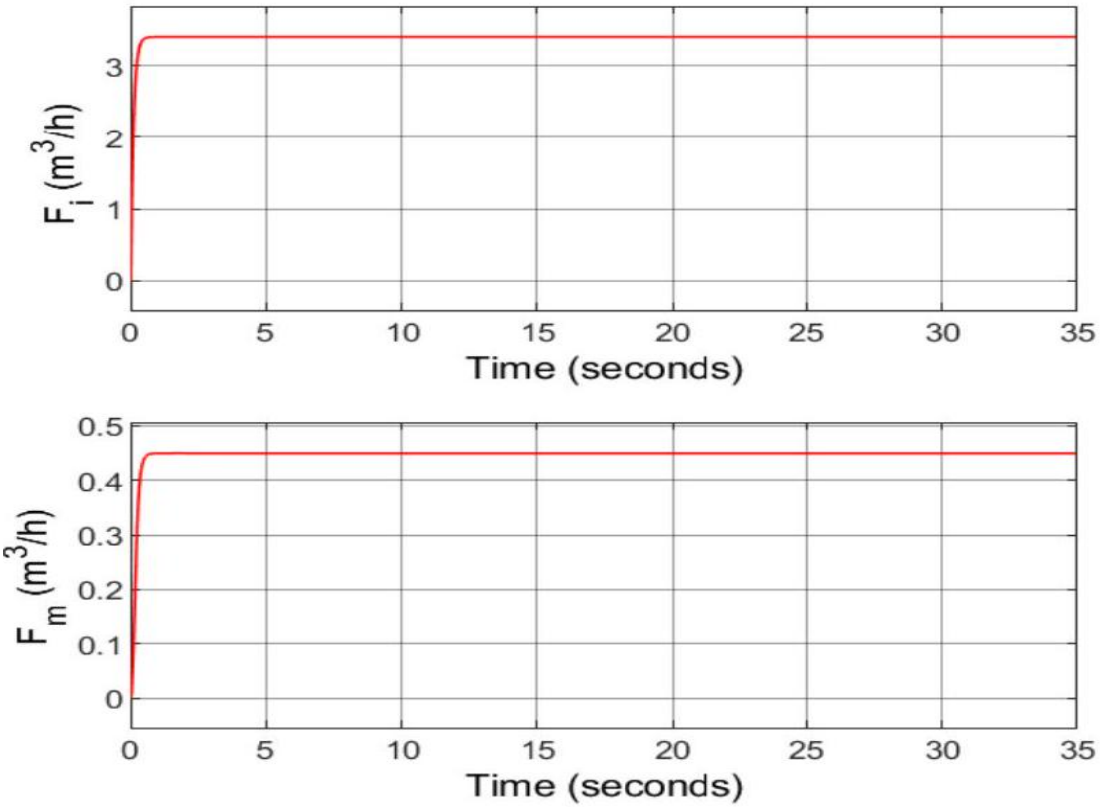

FIGURE 3: The inputs' responses

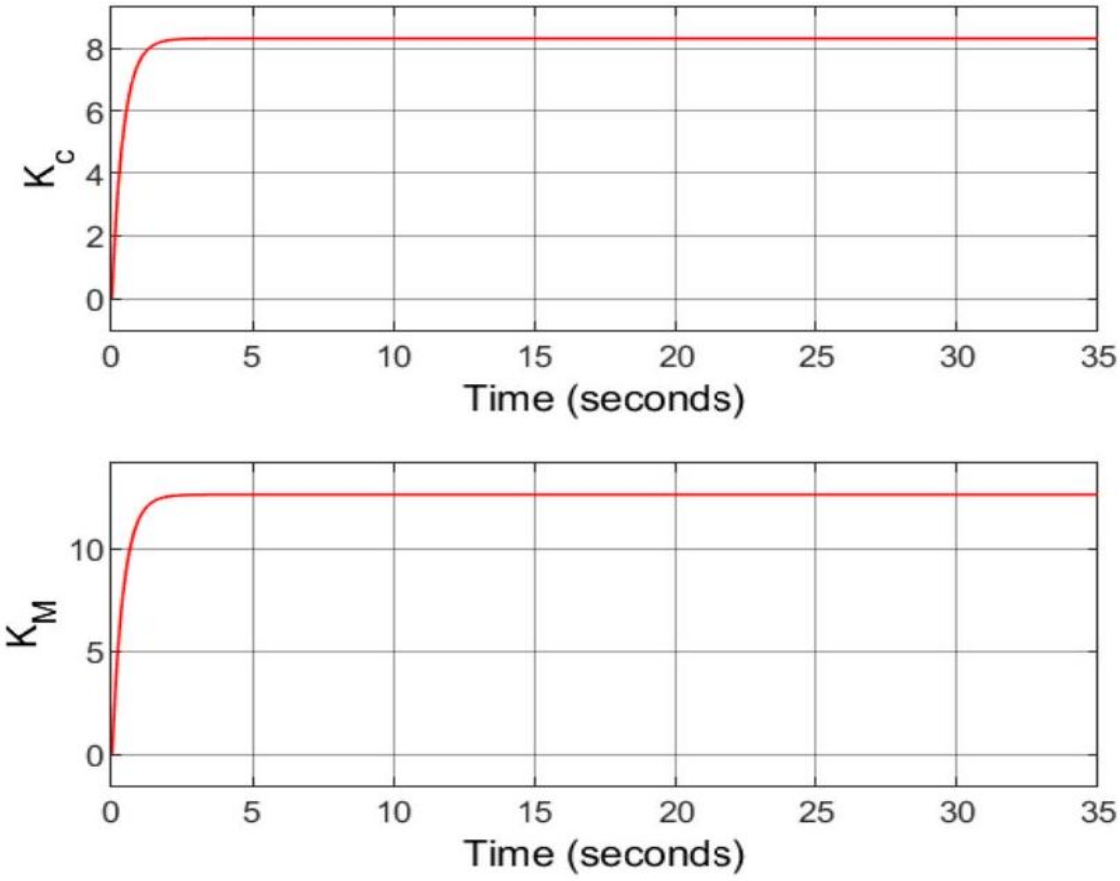

FIGURE 4: The upper bounds of the uncertainties

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