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ARTIFICIAL INTELLIGENCE FEATURES ON OBSERVATIONS OF NONLINEAR CHEMICAL REACTOR DYNAMICAL PROCESS

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This paper proposes a novel approach for enhancing the optimization of nonlinear high-gain observers by utilizing a genetic algorithm (GA) to improve state estimation precision in chemical reactors. Unlike traditional tuning methods, the GA optimally seeks optimal observer gain parameters that yield a minimum estimation error and improve convergence rates. The new method is used to benchmark a nonlinear continuous stirred-tank reactor (CSTR) model. The simulation outcomes validate that the GA-optimized observer exhibits a substantially enhanced rate of convergence and accuracy in estimating the temperature and concentration states compared to traditional methods. Additionally, the technique enables smaller dependence on physical sensors, thus promoting stronger and less expensive monitoring and control systems. The approach introduced is model-independent and applicable in real-time to an extensive class of engineering systems, including electrical and power systems. This work highlights the practical benefits of integrating metaheuristic optimization and nonlinear observer design in industrial processes.

1. INTRODUCTION

Artificial Intelligence (AI), especially when combined with machine learning and metaheuristic optimization, has become a powerful enabler of advanced estimation and control strategies for nonlinear dynamic systems. In the context of the chemical process industries, AI-based approaches significantly contribute to automating complex tasks and enhancing system performance through intelligent observer design and adaptive parameter tuning [1,2]. Recent contributions have highlighted the potential of hybrid metaheuristic algorithms integrated with deep learning to enhance estimation accuracy and computational efficiency. For example, Sumithra et al. [3] developed a dragonfly–whale–lion optimized deep neural network for accurately estimating software cost, effort, and time. In related work, Babu et al. [4] proposed a modular neural network optimized by the Cuckoo Search algorithm for effective fault classification in wind turbines, demonstrating the adaptability of such techniques to various nonlinear and dynamic environments. One of the classic issues with chemical reactors is the reliable estimation of internal states, particularly in nonlinear systems where sensor constraints, disturbances, and model uncertainty limit real-time monitoring. High-gain observers (HGOs) have been among the robust techniques employed for estimating unmeasured states from dynamic models and output measurements available [5–7]. They are based on gain amplification and are used to enable fast convergence of errors under any noisy or uncertain conditions. But the performance of an HGO is susceptible to the selection of its gain parameter. An HGO may converge very slowly or be very noise-sensitive if its gain is not adequately set. Conventional tuning procedures are often based on heuristic rules or even direct manual tuning and may be inadequate for nonlinear and time-varying operations. It is due to this reason that Artificial Intelligence tools, specifically GAs, prove to be a suitable alternative for automating gain selection [8,9]. GAs have been shown to possess global search capability and stability in solving challenging, non-convex optimization problems.

There has also been some recent research extending the use of HGOs to more complicated and organized systems. Ahmed-Ali et al. [10], for example, introduced an HGO-based output feedback control of nonlinear partial differential equation systems. Gerbet and Röbenack [11] designed a high-gain observer for polynomial dynamical systems for embedded control. Mousavi and Guay [12] proposed filtered multi-high-gain observer structures to solve estimation for multiscaling multi-phase dynamics systems. The contributions mentioned above indicate future lines of research in HGO methods for various types of systems. Our interest in this paper is in optimizing and designing a high-gain observer for a nonlinear continuous stirred tank reactor (CSTR). The CSTR is a highly tested benchmark system in observation and control experiments due to its nonlinear and robust dynamics, as well as its sensitivity to reaction kinetics [13,14]. Our novel contribution is adopting a GA to tune the observer gain independently, enhancing the convergence rate and accuracy of the estimated states (temperature and concentration), even in uncertainty and disturbances.

Simulation experiments confirm the proposed approach through the demonstration of enhanced estimation performance over conventional methods. The observer also substantiates state reconstruction without sensor infrastructure, hence being deployable for real-time implementations. The proposed framework is model-free and deployable in multiple disciplines, including electrical, energy, and environmental systems.

In addition to these developments, recent contributions published in the *Revue Roumaine des Sciences Techniques, Série Électrotechnique et Énergétique* have emphasized the integration of advanced control strategies with artificial intelligence and optimization methods. For instance, Roubache and Chaouch [15] investigated nonlinear fault-tolerant control approaches for electric vehicle drives, while Amrane et al. [16] proposed adaptive nonlinear control schemes for variable-speed wind turbines. More recently, Elumalai [17] investigated the application of neural network-based controllers to enhance power quality and tracking performance in renewable energy systems. A 2025

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study further advanced this trend by applying artificial neural networks for pitch angle control in wind turbines [18]. These works highlight the growing role of AI-driven and observer-based techniques across different energy and process domains, reinforcing their relevance for chemical reactor state estimation and control.

2. CHEMICAL REACTOR PROCESS MODEL

A chemical reactor is a process vessel designed specially to enable chemical reactions and is regarded as a unit operation of basic importance in chemical process analysis [13]. It is designed to create the optimal conditions for chemical conversion, including sufficient temperature, pressure, and proper mixing of the reactants. The design and operation of a chemical reactor are dictated by numerous factors, including the reaction type, the required yield of the product, and safety considerations [14].

There are several types of reactors, including batch reactors, plug-flow reactors (PFR), semi-batch reactors, and continuous stirred-tank reactors (CSTR) [19]. Batch reactors are typically used at the laboratory scale for measuring kinetics. In contrast, continuous reactors, such as CSTRs, are commonly employed in industrial applications, where reactants are fed continuously and products are removed simultaneously [13].

Some recent research has investigated chemical reactor performance from various perspectives. For instance, a process safety time-based design hypothesis was proposed for batch reactors [20]; multi-objective optimization methods have been proposed for batch processes [21]; and new control methods have been utilized in CSTR systems [22]. Here, we emphasize the model CSTR due to its extensive utilization in both environmental and chemical engineering. Otherwise known as the mixed flow reactor (MFR), back-mix reactor, or continuous-flow stirred-tank reactor (CFSTR), the CSTR incorporates ideal mixing conditions and thereby serves as a default reference point for observer and controller validation [23]. Our research aims to improve the estimation of unmonitored states, such as concentration and temperature, which are crucial for achieving optimal reactor performance and stability. Because the CSTR is nonlinear and measurements are constrained, we introduce an artificial intelligence-optimized high-gain observer framework to provide precise real-time state estimation despite disturbances and uncertainty. Emerging technologies in reactor modeling and regulation have also accentuated the need for accurate estimation techniques. For example, [24] offers multi-objective optimization of batch systems, while [25] suggests an improved control strategy for CSTRs. These technologies underpin the emerging trend towards model-based and observer-based methodologies in chemical process systems. In the next section, we introduce the mathematical model of the CSTR employed in this research as the basis for observer design and optimization.

Figure 1 illustrates the reactor structure and the observation system, including the proposed observer. This reactor is equipped with a double jacket through which a coolant fluid circulates, allowing the reactor's contents to be cooled.

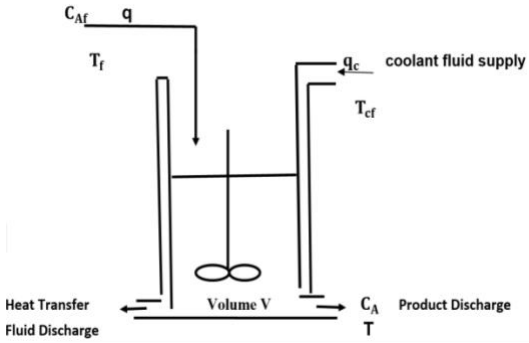

Fig. 1 – Schematic of a well-stirred continuous reactor (CSTR).

Table 1

Parameters

Variable/Parameter	Notation	Value
Feed flow rate	q	100 l /min
Feed concentration	C_{Af}	1mol/l
Feed temperature	T_f	350 K
Cooling temperature	T_{cf}	350 K
Reactor volume	V	100 l
Heat transfer coefficient	h_A	$7*10^5$ cal/min/K
Reaction rate constant	K_0	$7.2*10^{10}\text{min}^{-1}$
Activation energy	E/R	regular
Heat of reaction	ΔH	$-2*10^5$ cal/mol
Fluid densities	P, P_c	$1*10^3$ g /l
Specific heats	C_p, C_{pc}	1cal /g/k

The equations of the system are generalized in the following form [26]:

$$\begin{cases} \dot{C}_A = \frac{q}{v}(C_{Af} - C_A) - K_0 C_A \mathrm{e}^{-\frac{\mathrm{E}}{\mathrm{RT}}}, \\ \dot{T} = \frac{q}{V}(T_f - T) - \frac{\Delta H K_0}{P C_p} C_A \mathrm{e}^{-\frac{\mathrm{E}}{\mathrm{RT}}} + \frac{P_c C_{\mathrm{pc}}}{P C_{\mathrm{p}} V} q_C \left(1 - \mathrm{e}^{-\frac{h_A}{P_c C_{pc} q_C}}\right)(T_{Cf} - T). \end{cases} \quad (1)$$

where C_A, the concentration of the product at the outlet of the reactor, is the measured variable, q_c is the control variable, and C_{Af} is the disturbance. The model stands for the operating points C_A= 0.06, 0.1, and 0.13. The following table gives the results obtained for different values of C_{A}^0:

Table 2

Initial conditions.

C_{A}^0(mol/l)	0.06	0.1	0.13
T^0(k)	449.47	438.54	432.92
q_{c}^0(l/mn)	89.03	103.41	110.03

The dynamic process represented by:

$$\begin{cases} \dot{C}_A = \frac{q}{V}(C_{Af} - C_A) - K_0 C_A e^{\frac{-E}{RT}} = f_1, \\ \dot{T} = \frac{q}{V}(T_f - T) - \frac{\Delta H K_0}{P C_P} C_A e^{\frac{-E}{RT}} + \frac{P_c C_{\mathrm{pc}}}{P C_P V} q_C \left(1 - e^{\frac{-h_A}{P C C_P C q_C}}\right)(T_{Cf} - T) = f_2. \end{cases} \quad (2)$$

3. HIGH-GAIN OBSERVER DESIGN FOR CONTROL AFFINE SYSTEMS

Consider the general nonlinear system described by:

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \\ \mathbf{y} = \mathbf{h}(\mathbf{x}), \end{cases} \quad (3)$$

where $\mathbf{x} \in R^n$; $\mathbf{y} \in R^p$; $\mathbf{u} \in R^m$; $\mathbf{f}: R^n \times R^m \to R^n$, and $\mathbf{h}: R^n \to R^p$ are assumed to be smooth functions.

The transformed system appearing simpler, we will begin by designing an observer for system (3). We first write system (3) in a compact form for [27]:

$$\begin{cases} \dot{\mathbf{z}} = \mathbf{A}\mathbf{z} + \boldsymbol{\psi}(\mathbf{z}) + \boldsymbol{\Phi}(\mathbf{z})\mathbf{u}, \\ \mathbf{y} = \mathbf{C}\mathbf{z}, \end{cases} \quad (4)$$

where

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & & & 0 & 1 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix},$$

$$\boldsymbol{\psi}(\mathbf{z}) = \begin{pmatrix} 0 \\ 0 \\ . \\ . \\ . \\ 0 \\ \psi(z_1, \dots, z_n) \end{pmatrix},$$

$$\boldsymbol{\Phi}(\mathbf{z}) = \begin{pmatrix} \varphi(z_1) \\ \varphi(z_1, z_2) \\ , \\ . \\ . \\ \varphi(z_1, \dots, z_{n-1}) \\ \varphi(z_1, \dots, z_n) \end{pmatrix},$$

$$c = (1, 0, \dots\ 0).$$

Note that the nonlinearity $\boldsymbol{\Phi}(\mathbf{z})$ is said to be triangular. In effect, an observer for (4) is given by:

$$\dot{\hat{\mathbf{z}}} = \mathbf{A}\hat{\mathbf{z}} + \boldsymbol{\psi}(\hat{\mathbf{z}}) + \boldsymbol{\Phi}(\hat{\mathbf{z}})\mathbf{u} + k_\theta(\mathbf{y} - \mathbf{C}\hat{\mathbf{z}}), \quad (5)$$

where $k_\theta = \Delta_\theta k$ with $\Delta_\theta = \text{diag}\left(\frac{1}{\theta}, \frac{1}{\theta^2}, \dots, \frac{1}{\theta^n}\right)$ and $\theta > 0$, $\mathbf{K}$ is a matrix such that the matrix $(\mathbf{A} - \mathbf{KC})$) is stable. Now, we know that

$$\dot{\mathbf{z}} = \frac{\partial \boldsymbol{\Phi}(x)}{\partial x}\dot{\mathbf{x}} =$$

$$= \frac{\partial \boldsymbol{\Phi}(x)}{\partial \mathrm{x}}(\mathbf{f}(x) + \mathbf{g}(x)\mathbf{u}) \quad (6)$$

$$= \mathbf{A}\mathbf{z} + \psi(z) + \Phi(z)u$$

and

$$Y = h(x) + h(\Phi^{-1}(z)) = Cz. \quad (7)$$

On the other hand,

$$\hat{z} = \Phi(\hat{x}). \quad (8)$$

That is,

$$\dot{\hat{z}} = \frac{\partial \Phi(\hat{x})}{\partial x}\dot{\hat{x}}. \quad (9)$$

and therefore

$$\dot{\hat{x}} = \frac{\partial \Phi^{-1}(\hat{x})}{\partial x}\dot{\hat{z}} =$$

$$= \frac{\partial \boldsymbol{\Phi}^{-1}}{\partial x}(\hat{\mathbf{x}})[\mathbf{A}\hat{\mathbf{z}} + \boldsymbol{\psi}(\hat{\mathbf{z}}) + \boldsymbol{\Phi}(\hat{\mathbf{z}})\mathbf{u} + k_\theta(\mathbf{y} - \mathbf{C}\hat{\mathbf{z}})] = \quad (11)$$

$$= \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{g}(\hat{\mathbf{x}})\mathbf{u} + \frac{\partial \boldsymbol{\Phi}^{-1}}{\partial x}(\hat{\mathbf{x}})(k_\theta(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}})). \quad (12)$$

Hence, in the original coordinates:

$$\dot{\hat{\mathbf{x}}} = \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{g}(\hat{\mathbf{x}})\mathbf{u} + \frac{\partial \boldsymbol{\Phi}^{-1}(\hat{\mathbf{x}})}{\partial x}(k_\theta(\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}})), \quad (13)$$

and $\mathbf{g}(\hat{\mathbf{x}})$ must be uniformly Lipschitz continuous.

A careful choice of the high-gain observer's design parameter should ensure a balance between fast convergence and robustness against measurement noise.

4. HIGH-GAIN OBSERVER SYNTHESIS OF CHEMICAL REACTOR PROCESS AND RESULTS DISCUSSION

The construction of a high-gain observer can be synthesized in the coordinate space z. To obtain the observer's equations in the original coordinates, it suffices to multiply the gain vector in the new coordinates $\Delta_\theta^{-1}\mathrm{k}$ by the inverse of the Jacobian transformation matrix $\frac{\partial \boldsymbol{\Phi}^{-1}}{\partial \mathrm{x}}(\mathbf{x})$.

AN:

$$\dot{C}_A = \frac{q}{100}(1 - C_A) - 7.2 \times 10^{10} \times C_A \times \exp\left(\frac{-10^4}{T}\right),$$

$$\dot{T} = \frac{q}{100}(350 - T) + 14.4 \times 10^{12} \times \mathrm{C_A} \times \exp\left(\frac{-10^4}{\mathrm{T}}\right) +$$

$$+ \frac{q_c}{100}\left(1 - \exp\left(\frac{-7 \times 10^2}{q_c}\right)\right)(350 - T), \quad (20)$$

$y_1 = C_A$, and $y_2 = T$.

For the system under consideration, the observer's equations in the original coordinates are detailed as follows:

$$\begin{cases} \dot{\hat{C}}_A = \frac{q}{V}(1 - \hat{C}_A) - 7.2 \times 10^{10} \times \hat{C}_A \times \exp\left(\frac{-10^4}{\hat{T}}\right) + \theta k_1(C_A - \hat{C}_A) \\ \dot{\hat{T}} = \frac{q}{100}(350 - \hat{T}) + 14.4 \times 10^{12} \times \hat{\mathrm{C}}_\mathrm{A} \times \exp\left(\frac{-10^4}{T}\right) + \\ \frac{q_c}{100}\left(1 - \exp\left(\frac{-7 \times 10^2}{q_c}\right)\right)(350 - \hat{T}) + \\ + \left(\frac{\frac{q}{100} + 7.2 \times 10^{10} \times \exp\left(-10^4/T\right)}{\frac{7.2 \times 10^{14}}{T^2} C_A \times \exp\left(-10^4/T\right)} \times \theta h_1 + \boldsymbol{\theta^2} K_2 \times \frac{T^2}{7.2 \times 10^{14} \times C_A \times \exp\left(-10^4/T\right)}\right) \\ (C_A - \hat{C}_A) \end{cases} \quad (14)$$

The gain $\mathbf{K}$ is chosen equal to: $\mathbf{K} = \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} 10 \\ 20 \end{pmatrix}$.

5. GENETIC ALGORITHMS OPTIMIZATION

A genetic algorithm (GA) is a sophisticated heuristic optimization technique rooted in the principles of natural selection and genetics. It leverages evolutionary processes, such as selection, crossover, and mutation, to iteratively refine a population of potential solutions to a given problem. In GA, a diverse set of candidate solutions evolves over multiple generations, with the fittest individuals selected to pass their genetic material to future generations. This iterative mechanism, driven by crossover and mutation, generates new solutions aimed at achieving the optimal or near-optimal solution [28]. Conceptually, GA treats optimization problems like ecosystems, where feasible solutions represent organisms within this environment. These solutions are encoded using binary strings or other symbolic formats from a predefined set. By mimicking natural evolutionary processes, GAs efficiently navigate complex, high-dimensional search spaces, often outperforming traditional optimization methods in terms of both robustness and solution quality [28].

The success of GAs in addressing complex problems is widely recognized across various fields. For example, GAs have been employed to enhance constrained learning path adaptations [29], optimize parameters in the quantum approximate optimization algorithm [30], solve flexible job

shop scheduling issues using hybrid methods [31], improve energy efficiency in 3D wireless sensor networks [32], and optimize logistics routes in township settings [33]. These applications highlight the versatile and robust nature of genetic algorithms in solving a wide array of challenging optimization problems.

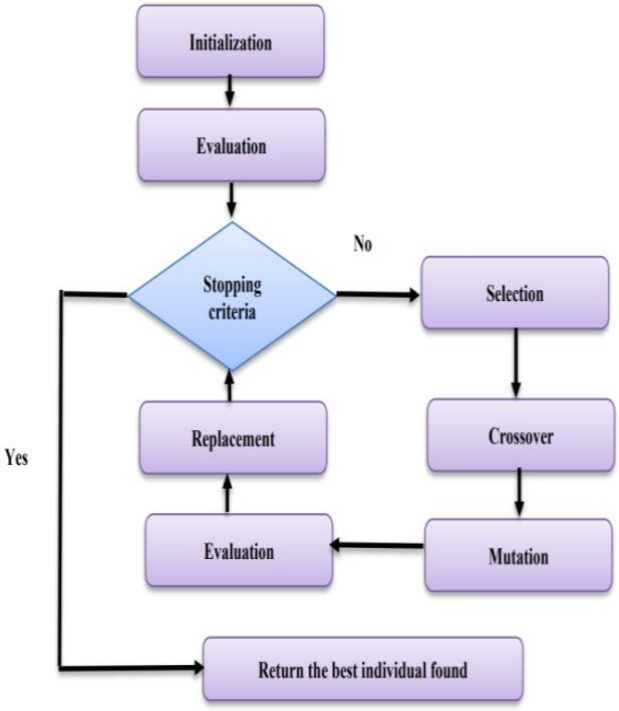

Fig. 2 – GA algorithm process.

The genetic algorithm is a procedure for optimization based on the mechanics of natural selection and natural genetics. It searches for solutions to complex problems by attempting to find an optimal or near-optimal solution through an evolutionary process. This consists of the following (Fig. 2):

1. Initialization: It begins with an initial population of candidate solutions, usually created quite randomly. Each chromosome encodes a potential solution to the problem in some coded form, most often in binary-coded form.

2. Fitness (Evaluation): The population of individuals is judged by their fitness with respect to the problem as measured by the appropriate fitness function. Selection has the consequence that 'good' solutions tend to survive, because individuals possessing better measures of fitness are more likely to be selected for reproduction.

3. Crossover/Reproduction: The reproduction or mating procedure is responsible for establishing the way in which individuals are allowed to mate. The standard selection methods include roulette (proportional to fitness), tournament, or rank, where the best individuals are favored to move to the next generation.

4. Crossover: Two selected parents exchange parts of their chromosomes to generate new offspring. Crossover (or recombination) introduces diversity into the population by combining the characteristics of both parents. Several crossover methods exist, such as single-point or multi-point crossover, or uniform crossover.

5. Mutation: It is the random change applied to the genes of the offspring chromosomes after crossover. It includes random changes in one or more parts of the chromosome to explore new solutions and prevent the algorithm from converging to local optima.

6. New Generation: The newly generated individuals, after selection, crossover, and mutation, will form a new generation. A cycle: With each new generation, better solutions in terms of survival are adapted.

7. Termination Criterion: The evolutionary process is continued until a stopping criterion is met or a stopping point, for example, a predefined number of generations or when the solution reaches a desired performance threshold.

The genetic algorithm constitutes a powerful method among metaheuristic methodologies used to search large-scale solution spaces to find the optimal solutions for complex problems. The use of its evolutionary mechanisms, including selection, crossover, and mutation, allows it to navigate successfully through high-dimensional search spaces, typically with higher robustness than conventional optimization techniques.

6. HIGH-GAIN GENETIC ALGORITHMS OPTIMIZATION OBSERVER

The application of the GA for optimizing the observer gain parameter θ has proven highly effective, achieving fast convergence and near-zero estimation error. The GA successfully identified the optimal θ value, which is crucial for the high-gain observer's performance.

In the simulations, the performance index was evaluated using the integral of time-weighted absolute error (ITAE), which emphasizes both rapid convergence and the minimization of long-lasting estimation errors.

Figure 3 illustrates the best function achieved by the GA, demonstrating its effectiveness in determining this optimal parameter. In the system simulation using the high-gain observer with the optimal θ value of 3.290885556070827 (as calculated by the GA), superior results were obtained.

Figures 4 and 5 show that with this optimal θ, the observer quickly converges to the actual state of the process while keeping the parameter low enough to provide accurate estimates for the variables CA and T. Figures 6 and 7 further demonstrate the minimal error between the real and estimated states for CA and T, respectively, confirming the high accuracy of the observer with the GA-optimized parameter. Compared to traditional methods for calculating observer gains, the GA-based optimization method not only offers superior accuracy and rapid convergence but also significantly reduces computational complexity and processing time. Overall, GA optimization demonstrates its efficiency in enhancing observer performance and optimizing gain parameters for precise state observation, thereby underscoring the advantages of artificial intelligence-based algorithms in modern control systems.

Table 3

Optimization algorithm parameter settings

	GA
Population size	50
Generations	25

Table 4

Optimal Parameter

Parameters	Optimal parameter
Theta parameter θ	3.290885556070827

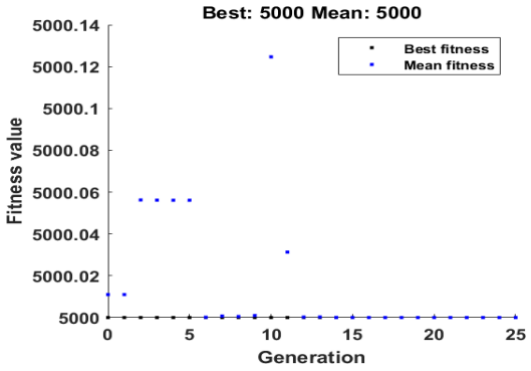

Fig. 3 – Genetic Algorithm best function.

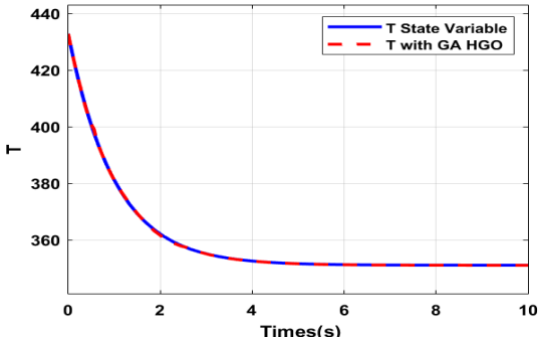

Fig. 4 – The Evolution of the estimated and actual state variables T with GA optimization.

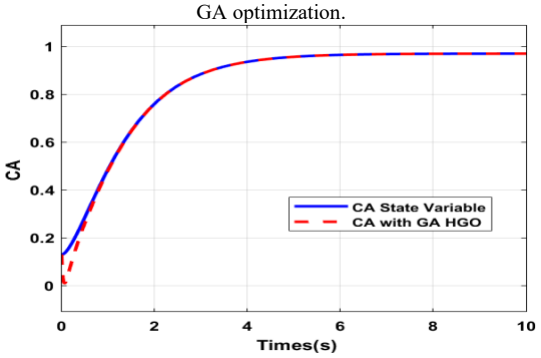

Fig. 5 – The Evolution of the estimated and actual state variables CA with GA optimization.

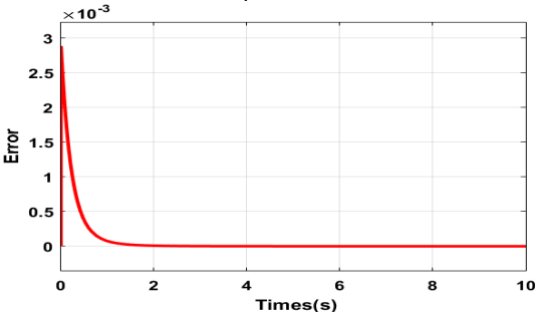

Fig. 6 – The Evolution of the error between estimated and actual state CA.

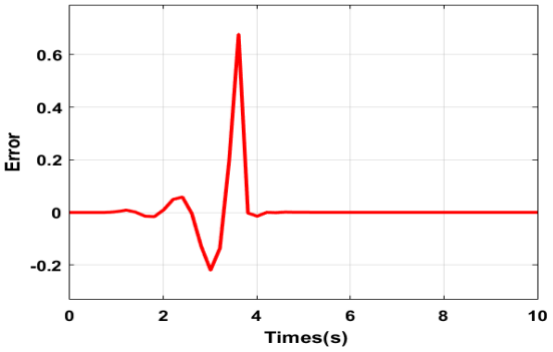

Fig. 7 – The Evolution of the error between estimated and actual state T.

7. CONCLUSIONS

In conclusion, the potential of a high-gain observer with an optimally designed gain parameter, as determined by a genetic algorithm, has been demonstrated in this work. Taking advantage of the capability of the GA to search complex and nonlinear solution spaces, we were able to compute the optimal value of the gain (θ) that resulted in fast convergence and negligible estimation error in a nonlinear chemical reactor process. When compared to conventional observer tuning approaches, the proposed strategy offers significant improvements in robustness, estimation accuracy, and computational efficiency.

The continuous stirred tank reactor (CSTR) was chosen as a representative nonlinear benchmark to test the observer design. The experiment verifies that adding AI-based optimization, specifically the application of a genetic algorithm, can improve performance on nonlinear observers without requiring extra sensors or model simplification.

Future studies can involve the extension of this methodology to other reactor configurations like plug flow or semi-batch operations, and investigation of hybrid metaheuristic techniques with the combination of GAs with ant colony optimization or neural-based learning. Additionally, the incorporation of adaptive machine learning algorithms for online adjustment of observer parameters can also make autonomous, scalable, and innovative process monitoring and control a reality in the process industry.

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CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Souaad Tahraoui: conceptualization, methodology, supervision, writing – original draft preparation, writing – review and editing.
Habiba Houari: data curation, validation, formal analysis, writing – review and editing.
Maamar Souaihia: software implementation, simulation, visualization, and investigation.
Hakima Mostefaoui: resources, literature review, writing, review, and editing.
Rachid Taleb: project administration, funding acquisition, supervision.
Elhadj Bounadja: formal analysis, model development, validation.
Youssouf Mouleloued: data collection.

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