

Identification of the Tennessee Eastman Chemical Process Reactor Using Genetic Programming

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Abstract

The Tennessee Eastman chemical process is a well-defined simulation of a chemical process that has been commonly used in process control research. As chemical process plants are getting more complex, the pressure on chemical engineers to develop accurate models for monitoring and control purposes is increased. In this paper, we explore the idea of using Genetic Programming (GP) technique to model the Tennessee Eastman (TE) Chemical Process Reactor. The process is decomposed to four subsystems. They are reactor level, reactor pressure, reactor cooling water temperature, and reactor temperature subsystems. GP found to have many advantages over other techniques in developing an automated process for industrial system modeling. A comparison between the applications of GP in modeling the TE chemical reactors subsystems with respect to other soft computing techniques such as Artificial Neural Networks (ANN), fuzzy Logic (FL) and Neuro-Gas and Neuro-PSO is provided.

Keywords: *Tennessee Eastman chemical process, Artificial Neural Networks (ANN), fuzzy Logic (FL) and Neuro-Gas and Neuro-PSO*

1. Introduction

There are many wide domains of applications in both scientific and engineering areas which depend on the development of a mathematical model which can be used for monitoring and control purposes. Industrial process is part of these challenging applications [1]. Applications such as parameter estimation, model optimization and process control are all in need for accurate simulation models which can help improving production quality, increase profit and minimize costs. Two techniques were proposed to handle the modeling problem of industrial nonlinear processes. The conventional method depends on constructing an automaton model based on facts of the fundamental physical (*i.e.* empirical) and chemical processes characteristics. In many cases, this method fails or provides inaccurate results due to the tremendous complexity of the system which makes it hard to be derived from the first principles analysis. In some cases, the developed mathematical model is poorly understood [2, 3]. The unconventional method is based on experimental data modeling. This method attempts to develop a process model which relies on minimizing the error difference between a target output and the original system output. On doing this a set of process variables are used as inputs to the model [4, 5].

In the past, models for linear systems were adopted to many industrial processes with various assumptions on the model. However, for complex industrial processes such as the TE process reactor innovative techniques are urgently required. Recently, many soft computing techniques were used to handle the modeling problem for industrial and chemical processes [6].

ANN was used to model the dynamics of nonlinear chemical process. A neural network learning algorithm of chemical process modeling based on the extended Kalman filter was presented in [7]. ANN based control strategies applied to a chemical reactor process was presented in [8]. The control objective was to force the operation of the system into a specific optimal trajectory. It is achieved by; manipulating coolant flow rate and the influent concentration. The resulting ANN models were cost effective compared to empirical models. Interested reader can find more details on the application of ANNs in modeling and control of nonlinear processes in [9–14]. Although the ANN approach has high prediction power in modeling dynamic systems, ANN has some disadvantages. ANN's structure has to be predetermined by the designer. In most cases, specifying an optimal structure as a setup would be a very hard task. Another disadvantage is that ANNs work as a black box prediction system. They fail in giving an explanations for their solutions [4].

A fuzzy logic based on Takagi-Sugeno method was used to generate an IF-THEN rules models of the TE chemical reactor's subsystems [15]. A set of generated fuzzy rules are used to model the dynamics of the TE process reactor. The characteristics of the predicted reactor level and pressure were very close to the actual output. These results indicate that the FL method has learned to model the dynamics of the level and pressure quite accurately. Authors in [16], proposed a comparison in evolving ANN weights using Particle Swarm Optimization (PSO) and Genetic Algorithms as a mechanism to improve the performance of ANN in modeling the TE chemical process. It was found that this approach is particularly useful in cases involved changing operating conditions as well as highly nonlinear processes. Evolved ANN based PSO outperform that one evolved using GAs.

Genetic programming was presented by J. Koza [17–19] at Stanford University in 1991. GP is part of the famous evolutionary computation techniques [20–23] which provide a methodology for the computer to solve wide domain of problems automatically. GP started with simple mechanism on solving problems based on simple LISP expression. Today, GP evolved rapidly, with novel techniques and applications. GP was explored by engineering community to solve diversity of problem in system identification and control. A computer program called Evolutionary Computation System Identification (ECSID) which automates the system identification process using Genetic Programming and Gene Expression Programming was presented in [24]. ECSID uses a function set, and observed data to determine an Ordinary Differential Equation (ODE) whose behavior is similar to the observed data.

The application of GP in nonlinear an model predictive control modeling got much interest in the past years. Authors in [25] showed that GP approach can be used to model discrete-time dynamic controllers that offer competitive performance for a specific class of control objectives. This work explains how GP is able to model dynamic recursive controllers for two example simulated processes: an Auto-Regressive eXogeneous (ARX) system and a simulated non-linear Continuous Stirred Tank Reactor (CSTR). Later on, authors in [26] described the application of genetic programming in modeling two empirical dynamic processes, a mixing tank and Karr liquid-liquid extraction column. They showed how GP can be deployed in both nonlinear and model predictive control strategy. These previous studies highlighted the power of GP approach in capturing the important features of the data into relatively simple analytical formulations.

In this paper, we propose the use of GP to build a new mathematical model for the Tennessee Eastman chemical process reactor. TE process, as presented by Downs and Vogel in [27], is based on an actual system, with slight changes made to protect the identity of the reactants and products. The system is a well posed problem for analysis and control design of a nonlinear, open-loop unstable chemical process [28]. In our experiments, the best evolved

model with minimum modeling error will be selected at the end of the evolutionary process. The GP based models will be compared with other presented models in the literature such as Artificial Neural Networks [4, 5], Fuzzy Logic (FL) [15], hybrid Neuro-genetic Algorithms and hybrid Neuro-Particle Swarm Optimization (PSO) [16] models.

2. Tennessee Eastman Process Description

The Tennessee Eastman Process (TE process) is a plant wide process control problem proposed by [27] as a challenge test problem given in Figure 1. TE process, as presented by Downs and Vogel in [27], is based on an actual system, with slight changes made to protect the identity of the reactants and products. The process consists of a two-phase reactor, a flash separator, a recycle arrangement, and two additional byproduct reactions. The TE process model is an open loop unstable process without control it reaches shutdown limits within an hour, even for very small disturbances [28]. A large number of interacting process and manipulated variables are incorporated into the model, making it a truly significant plant-wide control problem [29]. For more details about the TE chemical process see [30, 31]. The TE system is a well posed problem for analysis and control design of a nonlinear, open-loop unstable chemical process. The plant consists of five major operations: a two phase reactor, a product condenser, a vapor/liquid separator, a recycle compressor, and a product stripper. The nonlinear dynamics of the plant are mainly due to the chemical reactions within the reactor. The TE Chemical reactor process, given in Figure 2, was simulated for control purposes in [5, 28, 30].

3. System Identification Procedure

System identification field of research frequently uses statistical techniques to build mathematical models of dynamical systems using sets of measured data. Identifying the structure of nonlinear dynamical systems must be achieved by the following two major steps:

1. Choosing a model structure with a limited number of parameters and
2. Choosing an appropriate algorithm to estimate these parameters.

The conventional system identification process normally consists of number of steps which must be followed to achieve a minimum modeling error. The process can be summarized as follows:

- 1. Experimental data:** Collect input-output data from the process to be identified.
- 2. Select a class of models:** Define a set of candidate models within which the best model can be found as given in Equation 2. The general class of GP model structures using the output vector $y(t)$ is given by Equation 1. ϕ is the function which describe the system model and θ is the model parameters. t is the time instances, n_A is the maximum allowable delay in time for the output y and n_B is the maximum allowable delay in time for the input u .

$$y(t) = \phi(y(t-1), \dots, y(t-n_A), u(t-1), \dots, u(t-n_B), \theta)^T \quad (1)$$

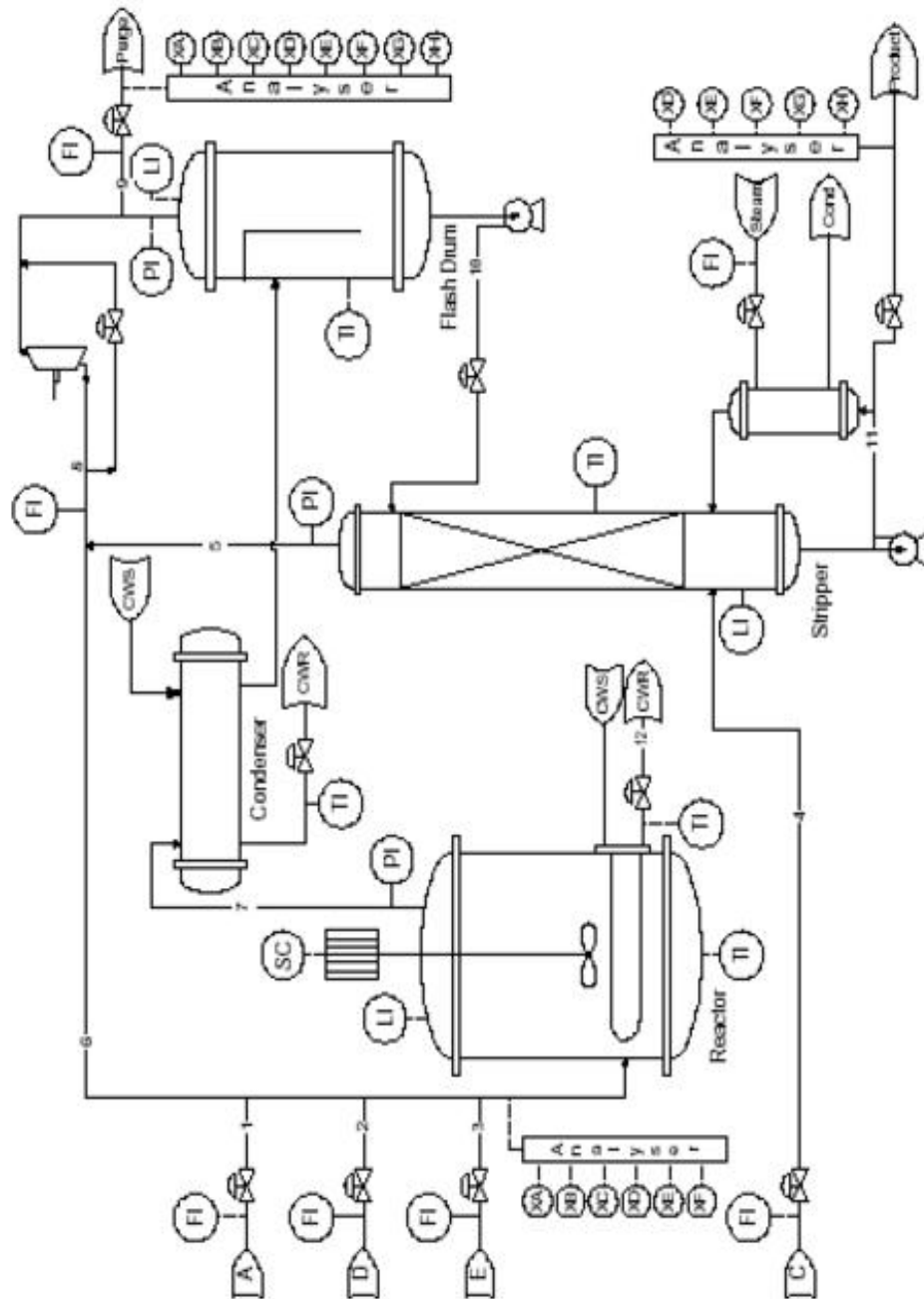


Figure 1. Tennessee Eastman Chemical Process [27, 30]

3. Select a model structure: Selecting a model structure from a set of candidate models is a difficult task since the TE reactor is a nonlinear process. The TE chemical process reactor has four main inputs $u_1(t)$, $u_2(t)$, $u_3(t)$, and a past output value $y(t-1)$ as given in Equation 2.

$$y(t) = \phi(y(t-1), u_1(t), u_2(t), u_3(t), \theta)^T \quad (2)$$

4. Model estimation: This stage concerning about estimating the model parameters and checking the developed model's properties. In our case, GP will be able to estimate the function ϕ and the model parameters θ .

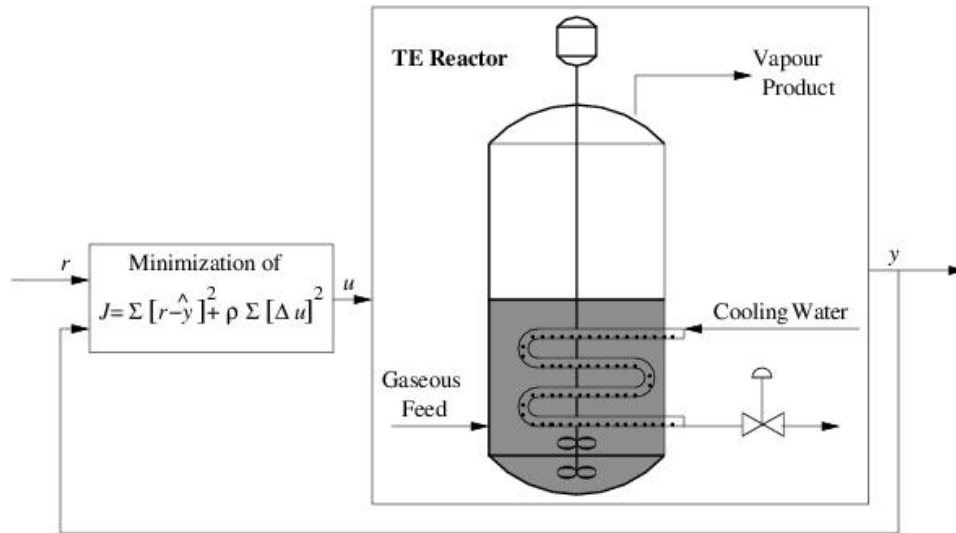


Figure 2. A Closed Loop Reactor System for Control Purposes [32]

5. Model validation: If the model is good enough, then we stop the evolutionary process; otherwise we go back and try another model structure. In order to check the performance of the developed regression model and compare the results obtained with previous works, the Variance-Accounted-For (VAF) performance criterion is measured. The VAF is computed as given in Equation 3.

$$VAF = \left[1 - \frac{\text{var}(y - \hat{y})}{\text{var}(y)} \right] \cdot 100\% \quad (3)$$

where y , \hat{y} are the actual output and the GP model estimated output, respectively. The VAF value between the estimated and the original output is performed to emphasize the capabilities of the proposed GP approach to model the TE process plant reactor and see how much it will be competitive to other approaches [33, 34].

4. Why Genetic Programming?

When modeling complex and dynamic processes such as Tennessee Eastman chemical process reactor in our case, the goal is not only to generate models that approximate the given target output value like in ANN, but also to give an insight on the dynamics of the underlying system [35]. Some unique advantages of GP models compared to empirical models [36] can be summarized as follows:

1. *Physical insight and understanding*: Models generated by GP can be interpreted by experts in the domain to identify underlying mechanisms and variables interrelationships.
2. *Simple summary models*: Models generated by GP are more simple and easier to evaluate compared to other softcomputing techniques like neural networks and support vector machines.
3. *Variable selection*: GP is able to identify the significant variables since they will appear more in the evolving models.

GP may not be the absolute superior method compared to some heuristic approaches [16]. However, GP has many advantages tempts to employ when modeling nonlinear system in the industry. GP generates models with interpretable structure, relating input and output variables from a data set without pre-processing and identifying key parameters. Therefore GP might shed insight into the underlying processes behavior and summarizes the interaction between input variables. Moreover, GP can identify the significant variables in any complex system since these variables will survive and appear in the best individuals (*i.e.* models) at the end of the evolutionary process [36]. For those reasons genetic programming approach was adopted to model the four chemical reactor sub-problems and can provide the advantage of the explanation power of this approach.

5. How Genetic Programming Works?

GP is an evolutionary approach that automatically generates and evolves computer programs in forms of mathematical models [17, 18]. Each of these models can be represented as a tree or as LISP expression. GP evolutionary cycle can be summarized in the following points:

- Initialization: GP starts by generating randomly a number of individuals (*i.e.* models) which form the initial population.
- Fitness evaluation: each individual is evaluated according to a specific measurement.
- Reproduction: in this process, a new population is created by applying the following three operations:
 - Selection mechanism: The mechanism used for selecting two individuals (*i.e.* parents) for reproduction. Usually the selection is based on fitness value of the parents.
 - Crossover: Creates two new individuals by exchanging and recombining randomly chosen subtrees from selected parents as shown in Figure 3.
 - Mutation: Creates new individual by replacing randomly chosen subtrees of an individual by another randomly generated subtree. An example of the mutation operation is shown in Figure 4.

- Termination of cycle: The evolutionary cycle starting from fitness evaluation point keeps iterating until an individual with certain fitness value is found or maximum number of iterations is reached.

6. Experimental Data

The quality and quantity of the training data is an important issue for GP modeling. Usually, the success of GP relies heavily on the amount of data, but this demand more computing time for training. In order to reduce the amount of data whilst maintaining the model quality, the data used must be carefully selected to ensure that they are sufficiently rich and avoid falling in the over fitting problem. The TE reactor modeling problem is divided into four sub-problems. They are: The reactor level, the reactor pressure, the reactor cooling water temperature, and the reactor temperature. Each of the four sub-problems has four input variables [4, 5, 16]. They are:

- f stand for the flow to the reactor.
- t stand for the coolant valve position,
- m stand for the feed mole fraction,
- p stands for the fourth delayed output $y_i(k-1)$, $i = 1, 2, 3, 4$. i represents subsystem number.
- The output of each sub-problem is named y_1, y_2, y_3 and y_4 .

Figures 5, 6, 7 and 8 show the three main inputs f, t , and m , and the output $y_i, i = 1, 2, 3, 4$ for each of the four sub-problems.

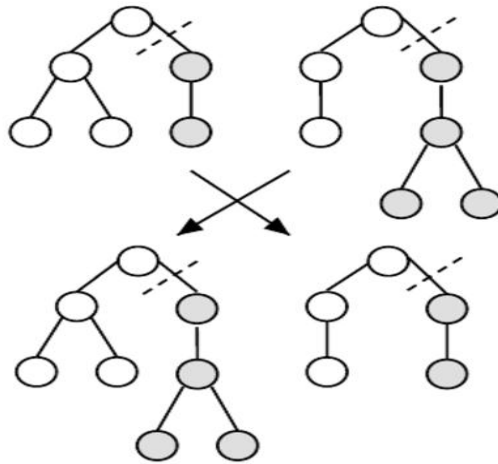


Figure 3. Example of the Crossover Operator

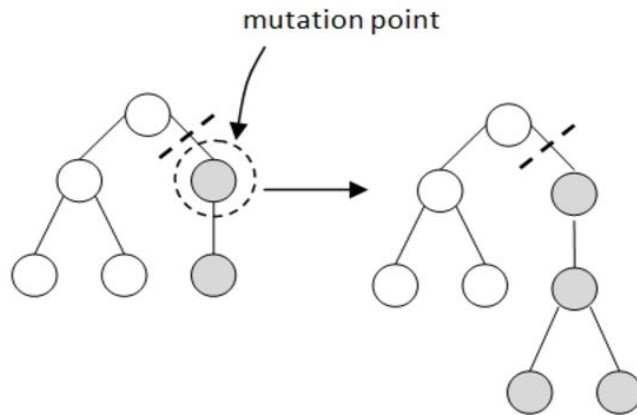


Figure 4. Example of the Mutation Operator

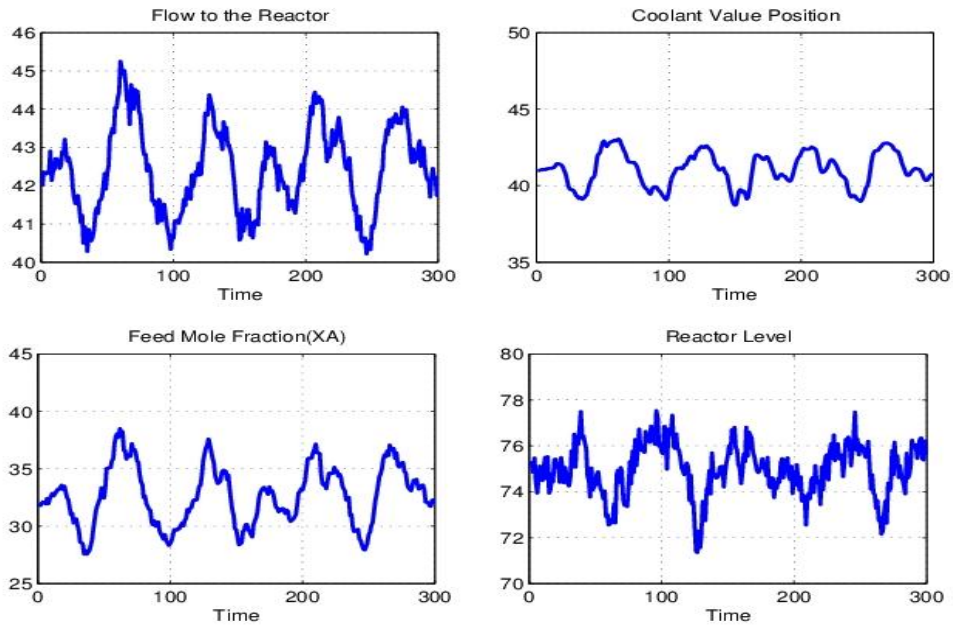


Figure 5. Input/Output Data for the Reactor Level Model

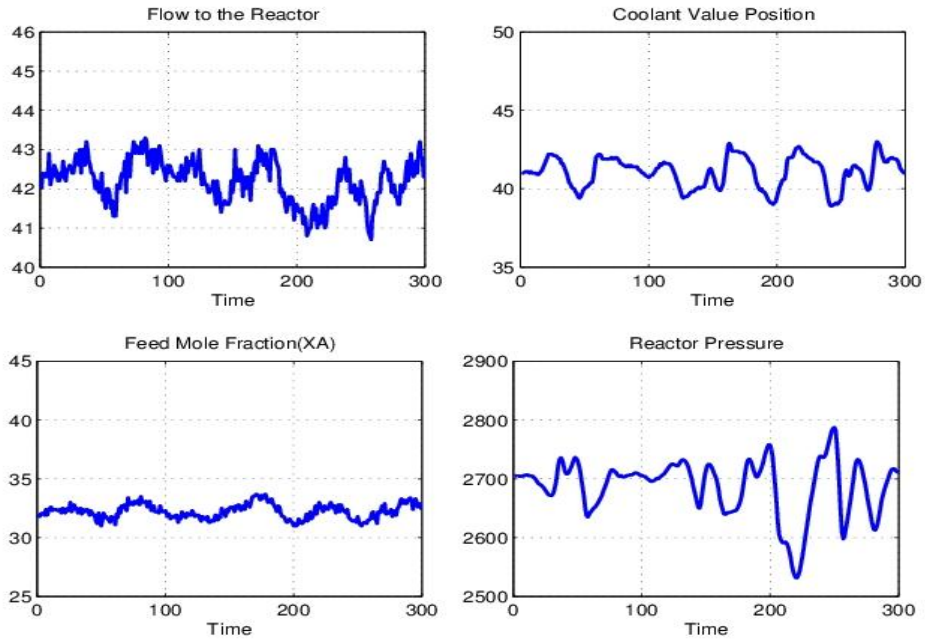


Figure 6. Input/Output Data for the Reactor Pressure Model

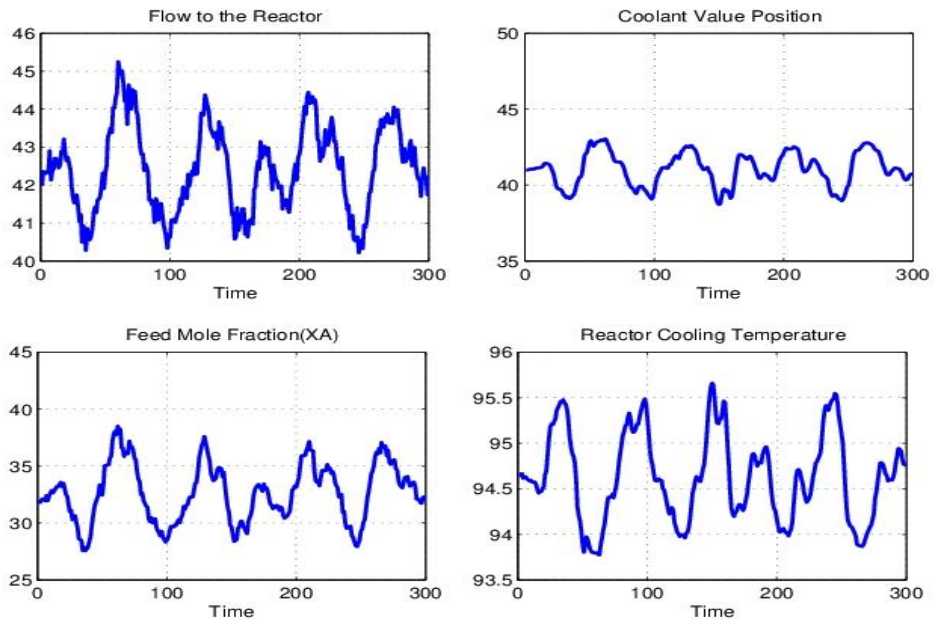


Figure 7. Input/Output Data for the Reactor Cooling Temperature Model

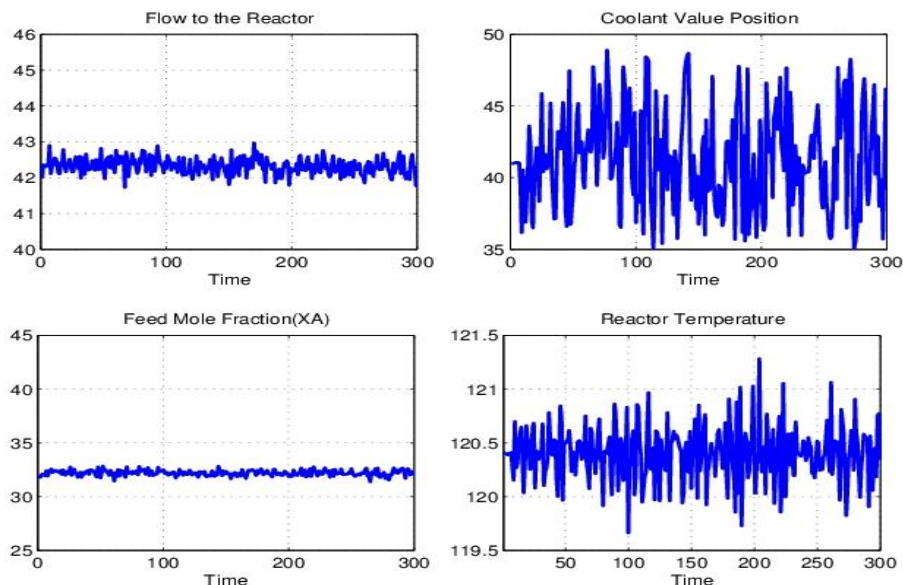


Figure 8. Input/Output Data for the Reactor Temperature Model

7. GP Experimental Setup

A symbolic regression model via genetic programming was proposed to model the dynamics of the four subsystems of the chemical process reactor. Only 300 data samples were used for both the training and validation phases. Data samples were downloaded from the online Tennessee Eastman Challenge Archive [37]. The data set describes the behavior of the TE reactor and shows how it responds to various inputs were collected under various operating conditions to measure different outputs of the reactor. The simulated data were split into two successive sets, each consisting of 150 data pairs. GP was used to build a model for the TE process using the first 150 data set (training set) while the next 150 data pairs (testing set) was used to ascertain the developed GP model.

Four different models were developed using the adopted GP parameters setting shown in Table 1 and four different function set for the f , t , m , and p . These function sets were chosen by many trial and error. i.e., different combinations of arithmetic operations (+, -, *, /) and mathematical functions such as (\sin , \cos , \exp , \log) were explored and tested to help finding the best model to improve the performance of the generated models. Choosing different sets of these operations for evolving GP generations can affect their quality and complexity. Therefore, select the best combination of the operations is a vital in the initial stage of the GP process.

In this study, we explored various function set for each subsystem model to determine the optimum set of mathematical operations of the GP model. Decision on the optimum topology was based on the minimum error produced in both training and testing cases. If this was successfully obtained, the model could safely be assumed as a reasonable representation of

the process data and hence the process itself. Due to random initial chosen sets, different runs produced different results.

Table 1. GP Symbolic Regression Parameters

Parameter	Value
Mutation probability	15%
Population size	1000
Maximum generations	10000
Selection mechanism	Tournament selector
Elites	1

8. Experimental Results

HeuristicLab framework¹ was used to simulate the experiments designed for the TE reactor subsystems. Four different sub-models, given in Equations 4, 5, 6 and 7, were developed using the GP parameters shown in Table 1. In Table 2, we show the computed VAF in both training and testing cases using GP for the four models developed. It is shown that GP managed to evolve four reactor sub-models with competitive performance accuracy compared to the ANN and FL models presented in [15, 38] as given in Table 3.

Table 2. VAF % Results for the Developed GP Models

Sub-problem	Training	Testing
Reactor Level	78.1076	56.5678
Reactor Pressure	59.8164	28.2841
Reactor Cooling	95.8191	95.7619
Reactor Temperature	99.8735	99.8125

In Table 3, the developed GP sub models managed to provide a significant enhancement over NNARX and FL by 4% to 50% for the reactor level and pressure, respectively. The results in terms of the reactor cooling temperature and the reactor temperature yield good results, meaning that those methods are highly stable towards the end. The four developed models are given in Equations 4, 5, 6 and 7. We used the symbols for the m for the feedMole, f for the flow and t for the coolant temperature. In Figures 9, 10, 11 and 12, the actual and estimated results of the genetic programming models for the Reactor Level, Pressure, Cooling and Temperature are shown, respectively. Figures 13, 14, 15 and 16 show the GP convergence process toward the best model. We can notice that in case of the reactor pressure model GP was slower to reach the best model. It converges after 1700 generations.

Comparing GP models with hybrid heuristic models show that hybrid approaches can outperform single optimization algorithm such as GP, ANN or FL alone. In Table 4, we compare the produced results using GP along with the results developed using Neuro-GAs and Neuro-PSO [16].

¹ HeuristicLab is a framework for heuristic and evolutionary algorithms that is developed by members of the Heuristic and Evolutionary Algorithms Laboratory (HEAL), <http://dev.heuristiclab.com>

Table 3. VAF % for the GP and Single Heuristic Models in Training Cases

Sub-problem	GP	FL[15]	NNARX [38]
Reactor Level	78.1076	68.5872	71.9788
Reactor Pressure	59.8164	46.4975	11.3203
Reactor Cooling	95.8191	97.7052	99.8723
Reactor Temperature	99.8735	99.9341	99.8174

Table 4. VAF % for the GP and Hybrid Heuristic Models in Training Cases

Sub-problem	GP	ANN-GAs[16]	ANN-PSO[16]
Reactor Level	78.1076	87.3228	90.9445
Reactor Pressure	59.8164	89.8116	91.9994
Reactor Cooling	95.8191	98.3863	99.7988
Reactor Temperature	99.8735	99.7300	99.9944

$$y_1 = (0.024 \cdot p + (0.717 \cdot m + \sin(14.32 \cdot m) \cdot \sin(0.219 \cdot m)) \cdot (-1) + \cos((0.768 \cdot m - 2.164 \cdot p)) + \sin((0.783 \cdot m - 1.071 \cdot p)) - 16.277) \cdot \sin(0.201 \cdot p) \cdot (-0.412) + 74.989 \quad (4)$$

$$y_2 = (0.0325 \cdot t + \cos(\sin(\tan(1.379 \cdot t))) \cdot 0.136 + \cos(\tan(\tan((1.984 \cdot t + 0.612)))) \cdot (-0.136) + \sin(\sin(\sin(-0.24 \cdot t))) \cdot 0.136 + \sin(2.009 \cdot p) \cdot 0.136 + \sin(\sin(\tan((1.984 \cdot t + 0.848)))) \cdot 0.136 + 118.958) \quad (5)$$

$$y_3 = (\tan(3.55 \cdot m) \cdot (2.196E - 05) + \tan(3.434 \cdot t) \cdot (-2.196E - 05) + m \cdot ((-0.582) \cdot t - \tan(\sin(\tan(3.78 \cdot t)))) + f \cdot \tan(3.483 \cdot p) \cdot 9.102 + (-123.577)) \cdot (2.181E - 05) + 2.81 \quad (6)$$

$$y_4 = \left(\frac{(-0.0416) \cdot m}{(0.0488 \cdot t - 16.084) \cdot (0.654 \cdot m - 16.182)} \cdot \frac{7.569}{0.655 \cdot f} \cdot ((-0.043) \cdot m - 16.084) - (16.526 - 0.326 \cdot t) \right) \cdot 1.298 + 90.324 \quad (7)$$

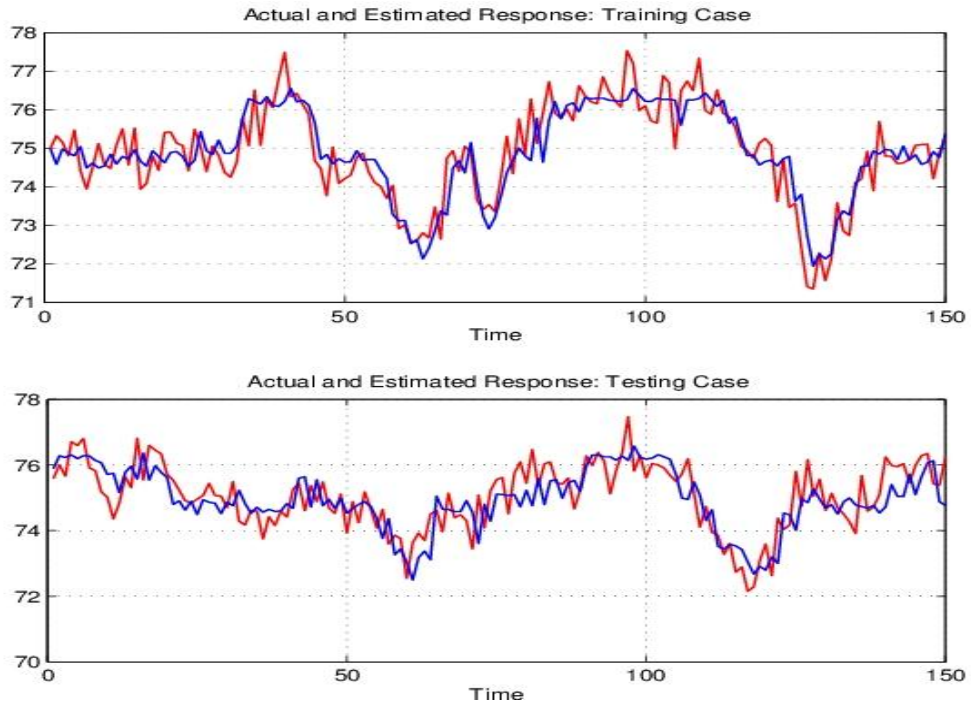


Figure 9. Observed Reactor Level and GP Model Responses (training and testing)

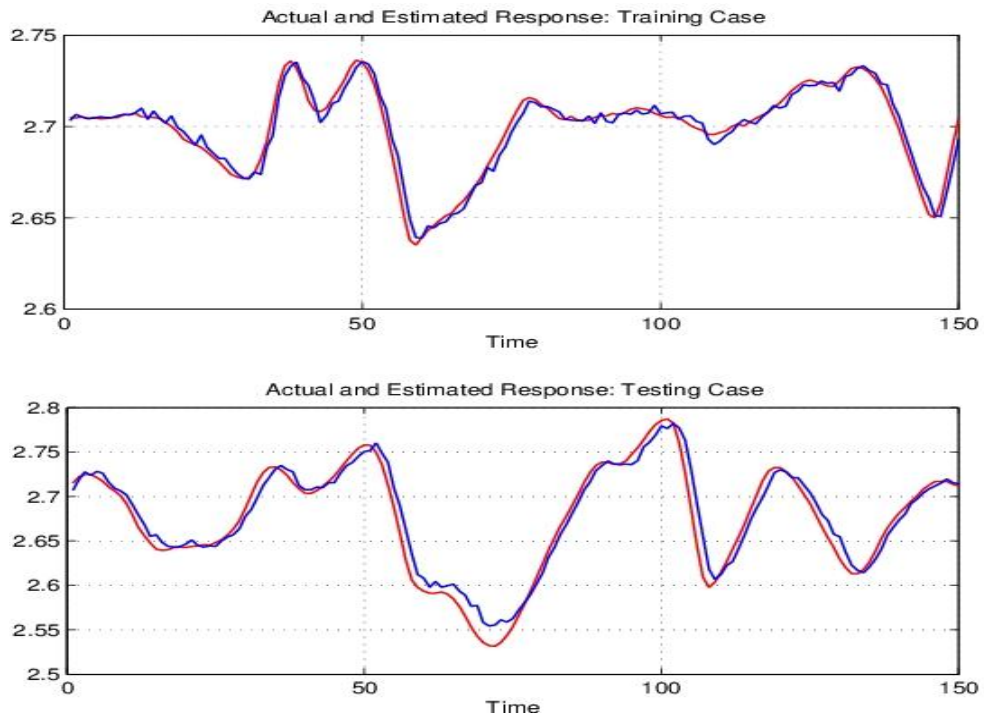


Figure 10. Observed Reactor Pressure and GP Model Responses (training and testing)

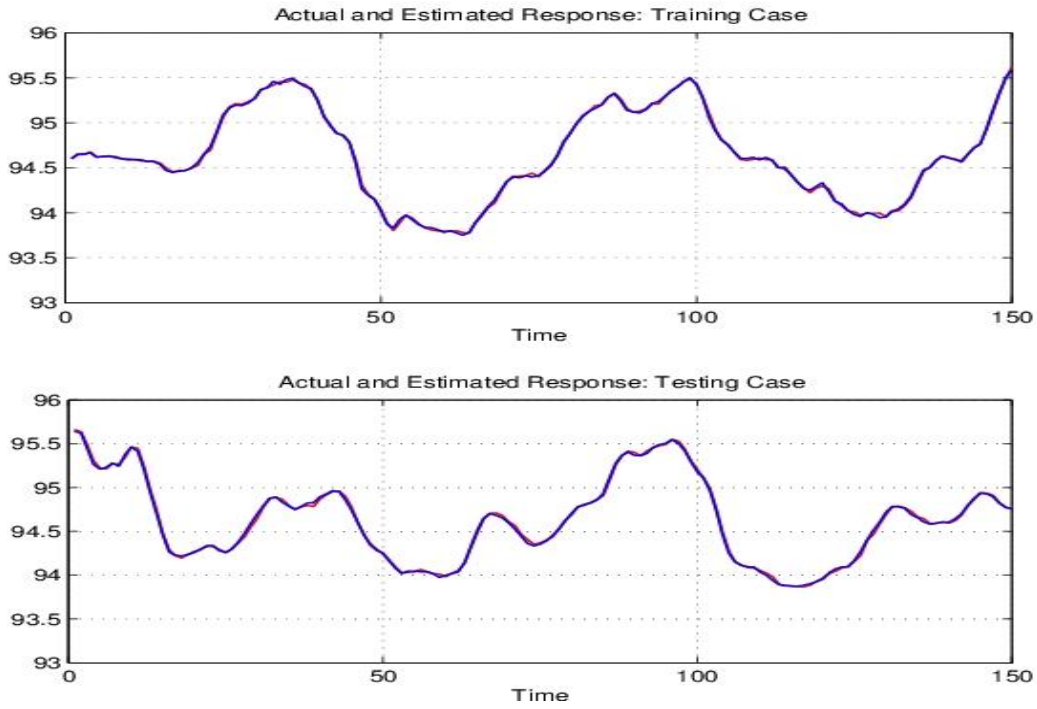


Figure 11. Observed Reactor Cooling Temperature and GP Model Responses (training and testing)

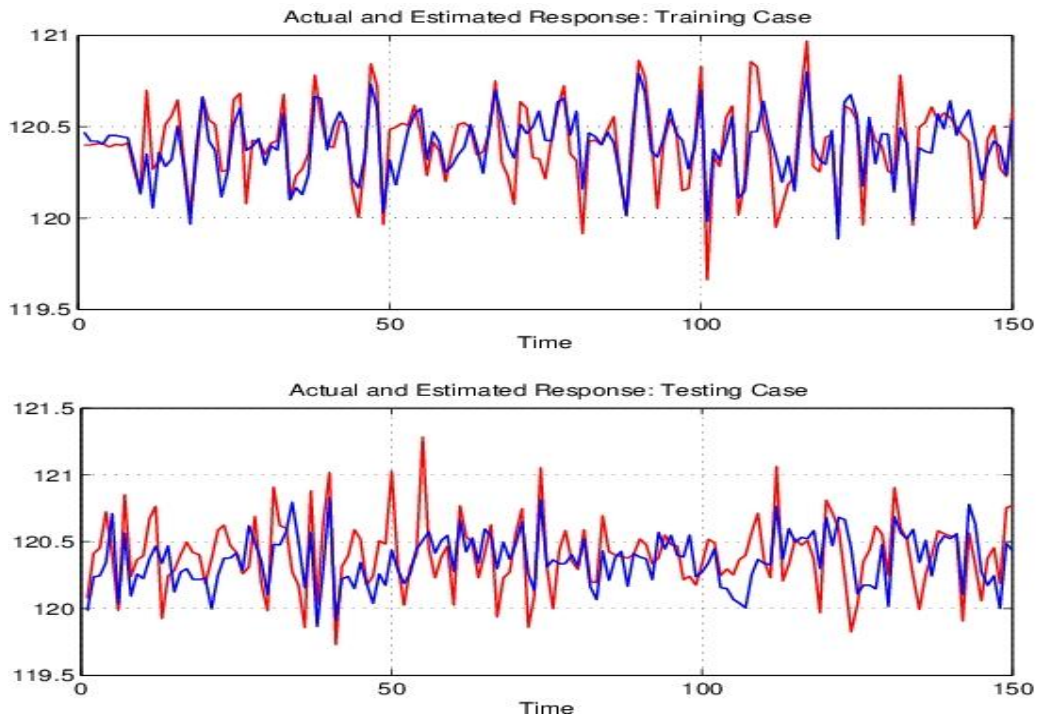


Figure 12. Observed Reactor Temperature and GP Model Responses (training and testing)

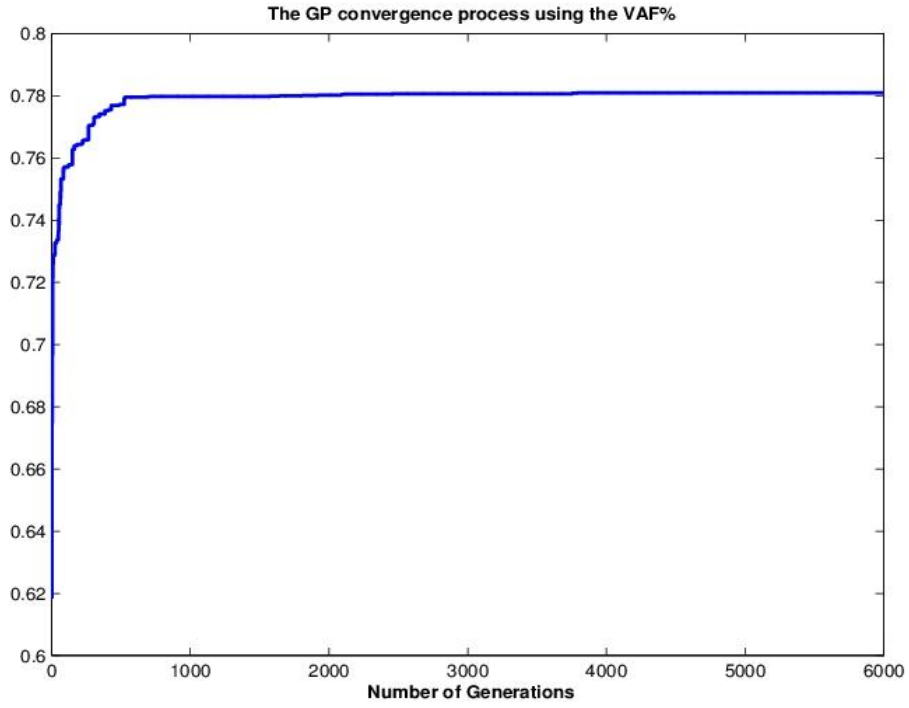


Figure 13. GP best so far for the Reactor Level Model

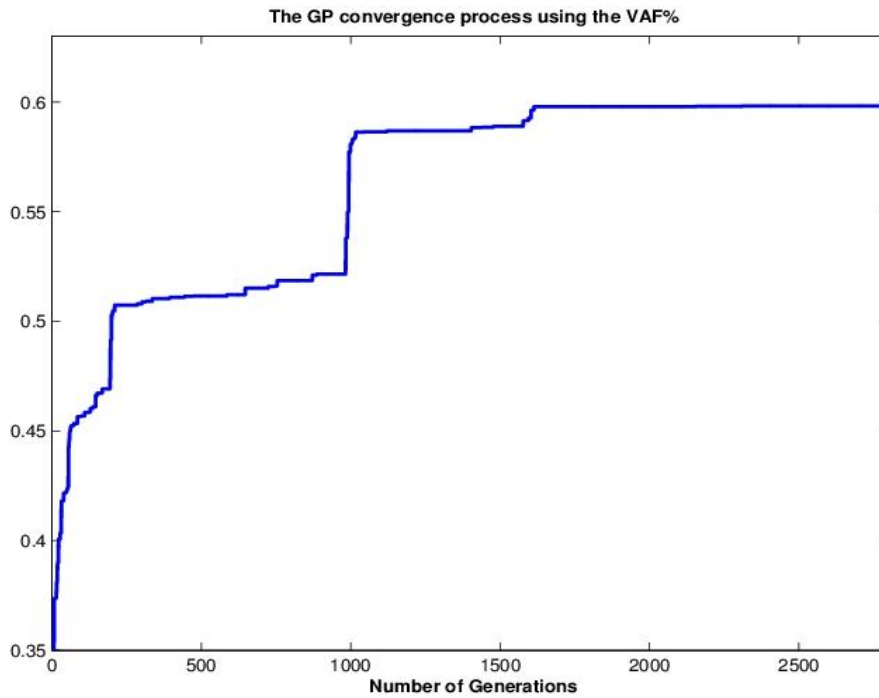


Figure 14. GP best so far the Reactor Pressure Model

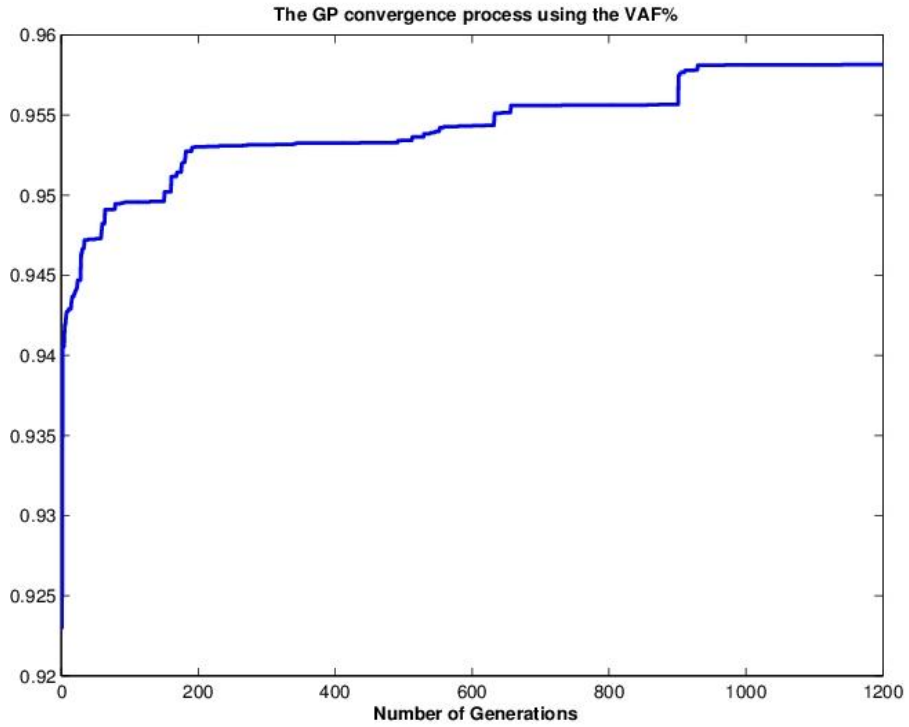


Figure 15. GP best so far the Reactor Cooling Temperature Model

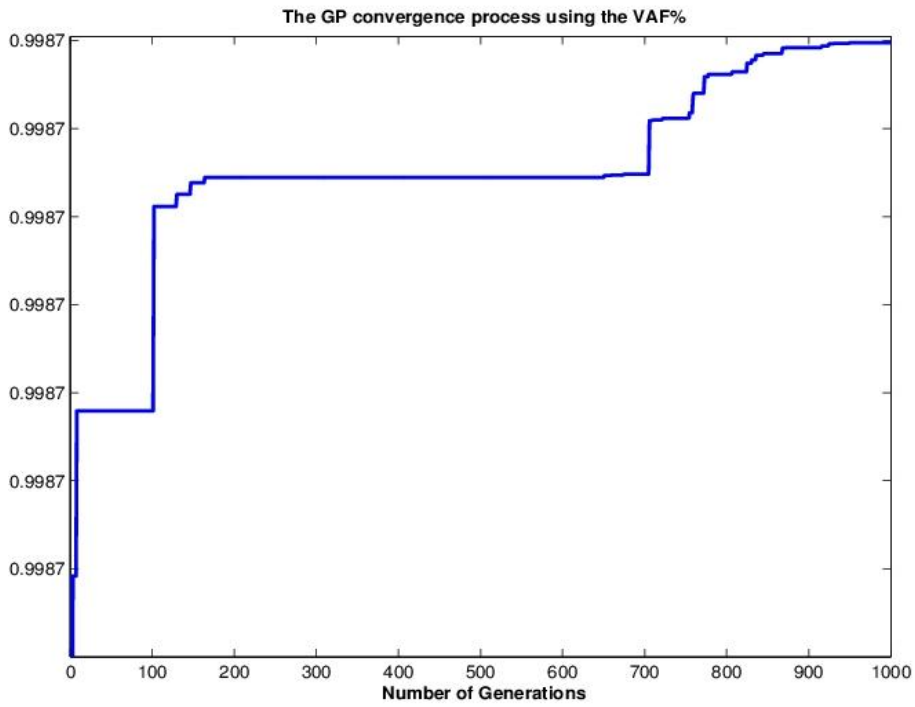


Figure 16. GP best so far the Reactor Temperature Model

9. Conclusions

In this paper, Genetic Programming was used to model the dynamics of TE chemical process reactor. GP showed the capability of finding accurate mathematical relationships for TE reactor subsystems: the reactor level, reactor pressure, reactor cooling water temperature, and reactor temperature.

The advantages of GP technique in developing an automated process for industrial system modeling were essential. The GP evolutionary model was compared with other soft computing techniques such as ANN, FL and also hybrid heuristic approaches such as Neuro-GAs and Neuro- PSO.

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