

Integration of Simulated Annealing and Pattern Search for Control of Distillation Process

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Abstract

This study presents the design of Simulated Annealing (SA) and Pattern Search (PS) based PID controller to control the reboiler temperature of multi-component distillation process. SA works on generation of test point in a vicinity of the present iterate and updates it by comparison of function values. The inappropriate cooling schedule of SA leads to sluggish conjunction rate and therefore a local search method i.e. hybrid of PS with SA is used to optimize PID parameters. SA provides fine initial parameters as a preliminary solution, then optimization shifts to PS algorithm to further improve the parameters value.

Three objective functions are considered out of which integration of absolute error is found suitable. The Genetic Algorithm tuned PID (GA-PID), Simulated Annealing tuned PID (SA-PID) and conventional PID controllers are also designed for the desired control purpose. It is observed from the results that SAPS-PID controller is robust and controls the product composition efficiently as compared to other designed Controllers.

Keywords: Distillation Column, Simulated Annealing (SA), Pattern Search, Genetic algorithm (GA), PID.

Introduction

The distillation is most widely used process in chemical industry. The prime objective of distillation process is to control the product quality in the facets of disturbances. In a chemical process, energy balance and material balance equations exhibit nonlinear characteristics thus making it highly nonlinear. Further dynamic equations describing chemical process have time dependent parameters, therefore a robust controller is required. Sometimes system variables and operating conditions change during the operation of chemical process which makes it difficult to control the process, so controller must adapt to the changes as quickly as possible and control the process efficiently.

The process considered for control purpose is a multicomponent distillation process. The quality of distillate product can be controlled using different control techniques; one of them is smart control mechanism.¹⁵⁻¹⁷ The traditional proportional-integral-derivative controller (PID) cannot achieve desired performance for such highly nonlinear, multifaceted and tentative processes. Due to these reasons, different tuning methods to determine the PID parameters

have been proposed in the literature. The most accepted tuning method is given by Ziegler-Nichols (ZN). These methods execute well for lower order processes but give average performance for higher order and non-linear systems.

An alternative approach is to optimize the parameters with the help of gradient-free optimization method such as Genetic Algorithm (GA), Simulated Annealing (SA), Tabu Search (TS), particle swarm optimization (PSO) used for control of distillation column. Other intelligent techniques like neural network (NN)^{13,14} are also used for control of chemical process. These methods are straightforward to apply and are not exaggerated by the higher order system environment and fitness function. Cardoso et al⁴ proposed a simulated annealing based algorithm for optimization of non-equilibrium reactive distillation column. This algorithm is capable of finding an optimal solution close to global optimum.

Wozny and PuLi¹⁹ used optimization techniques for the purpose of reducing startup time of distillation columns. Experimental results show reduction in startup time significantly after implementing the developed optimal policies. Miladi and Mujtaba¹¹ used SA for the optimization of design and operation policies of binary batch distillation with fixed product demand. Results show significant improvement in the annual profit. Cheng et al⁵ proposed SA based optimal steady state design of reactive distillation process. The SA-based optimization procedure gives an improved design than the best flow sheet obtained from the chronological design approach.

Zhong and Gang²² proposed a simulated annealing-based approach for synthesis of multi-component distillation system in which SA is adapted for mixed integer nonlinear programming (MINLP) optimization problems. Wang et al¹⁸ presented a paper on optimal operation strategies for batch distillation by using a fast adaptive simulated annealing algorithm. The results show the effectiveness of the proposed method.

Castillo et al⁶ presented the use of GA for optimization of intensified distillation systems for quaternary distillations. Results show that proposed design tool is robust and appropriate for the design of coupled multi-component distillation sequences. Yusof et al²⁰ proposed a technique based on GA and recursive least square method for fuzzy modeling based on the Takagi-Sugeno fuzzy model. Results show that this projected approach provides superior modeling when compared with linear modeling approach for process control application.

Domingues et al⁷ addressed the design of reactive distillation columns to produce ETBE based on detailed first-principles model which considers equilibrium and kinetic information, rigorous physical property data and catalyst deactivation. Two evolutionary techniques, GA and PSO have been used for this purpose. Results show that both algorithms are satisfactory to solve this design problem.

Singh et al¹⁵⁻¹⁷ presented three types of neural network-based control strategies i.e. NN-IMC, NN-DIC and NN-MRAC for the control of binary distillation column. Results show that NN-IMC strategy is superior in comparison to other controls.

Nisha and Pillai²⁴ proposed a nonlinear model predictive control strategy which utilize SVR and PSO with controllable random exploration velocity (SVR-PSO-CREV). Performance of proposed controller is then compared with NN-PSO-CREV based MPC for control of distillation column. Results show the superiority of proposed control strategy due to prediction accuracy of SVR in comparison to another controller. Baiesu²⁵ identified the local transfer function model based on markov parameter for nonlinear binary distillation column. Further obtained model is then validated by observing its performance for step change in input w.r.t actual model.

It is revealed from the literature that different intelligent techniques have been used for the design and control of various chemical processes. In order to utilize the benefits of Simulated Annealing and Pattern Search, a hybrid of these techniques is proposed to tune the PID controller for a multi-component distillation process, leading to SAPS-PID controller. In this paper SAPS optimizes various objective functions to achieve the best possible performance. GA-PID, SA-PID and Tyreus-Luyben tuned PID are also designed for the control purpose.

Modeling of distillation process

The multi-component distillation process under consideration¹⁰ has 15 trays, a reboiler to vaporize the mixture, a condenser to cool the overhead vapour and tray 5 is used as the feed tray. In distillation process, a liquid mixture of five components is fed on the feed tray and is stored in reboiler. The mixture is heated to produce vapour which rise from the bottom and after passing through stripping and rectifying section, condensed in the condenser. Initially the distillation column operates under total reflux condition in which the whole liquid from the condenser is refluxed back to the column.

During this condition, the lightest constituent is concentrated on the upper trays of the column whereas the concentration of the middle constituent and the heaviest constituent decreases in the top of the column. When the quality of the lightest constituent reaches its explicit purity level, then distillate product removal begins. The basic structure of distillation column is shown in figure 1. The mathematical

model of the distillation process with usual assumptions is as follows:

Component material balance equation for condenser

$$M_D \frac{dx_{Di}}{dt} = V_{NT} y_{NT} - V_{NT} x_{D,i}$$

Component material balance equation for reboiler

$$M_B \frac{dx_{Bi}}{dt} = L_1 x_{1,i} - V_B y_{B,i} - (L_1 - V_B) x_{B,i}$$

The component material balance equation for tray *k* is given by:

$$\frac{d(M_k x_{ki})}{dt} = L_{k+1} x_{k+1,i} - L_k x_{k,i} - V_k y_{k,i} + V_{k-1} y_{k-1,i} + F_k x_{Fki}$$

For *i* = 1, 2, …, *NC*; *k* = 1, …, *NT*

where *NT* = Number of trays, *NC* = Number of component, *M_k* = Molar liquid holdup on tray *k*, lb-mole, *x_{ki}* = Liquid fraction of component *i* leaving the tray *k*, %mole fraction, *L_k* = Total liquid flow rate leaving tray *k*, lb-mole/h, *V_k* = Total vapour flow rate leaving tray *k*, lb-mole/h, *F_k* = Total feed flow rate injected to tray *k*, lb-mole/h, *x_{Fki}* = Liquid fraction of component *i* in feed on tray *k*, %mole fraction.

The vapour composition of component *i* on tray *k* is obtained as:

$$y_{ki} = \eta_{ki} (y_{ki}^* - y_{k-1,i}) + y_{k-1,i}$$

where η_{ki} = Murphree stage efficiency based on vapour phase of component *i* on tray *k* and *y_{ki}^{*}* = Equilibrium vapour fraction of component *i* on tray *k*.

The total material balance for general tray *k* is calculated as:

$$\frac{dM_i}{dt} = L_{k+1} - L_k - V_k + V_{k-1} + F_k$$

The enthalpy balance for general tray *k* is given by the following equation:

$$L_{k+1} h_{k+1} - L_k h_k - V_k H_k + V_{k-1} H_{k-1} + F_k h_{Fk} = 0$$

Where *h_k* = Total molar enthalpy of liquid leaving tray *k*, kJ/lb- mole and *H_k* = Total molar enthalpy of vapour leaving tray *k*, kJ/lb-mole.

Enthalpies of liquid and vapour on tray *k* are calculated by mixing rule and are given by:

$$h_k = \sum_{i=1}^{NC} h l_{ki} x_{ki}$$

$$H_k = \sum_{i=1}^{NC} H v_{ki} y_{ki}$$

where h_{ki} and H_{vki} represent unadulterated component enthalpies of component i on tray k in liquid and vapor phase respectively. The mathematical model discussed above is simulated in Intel® Core™ i5 CPU with 2.4 GHZ frequency

and 4 GB RAM in MATLAB version 8.0.1.604. Figure 2 shows the simulation chart for multicomponent distillation process. All the governing parameters are given in Appendix A.

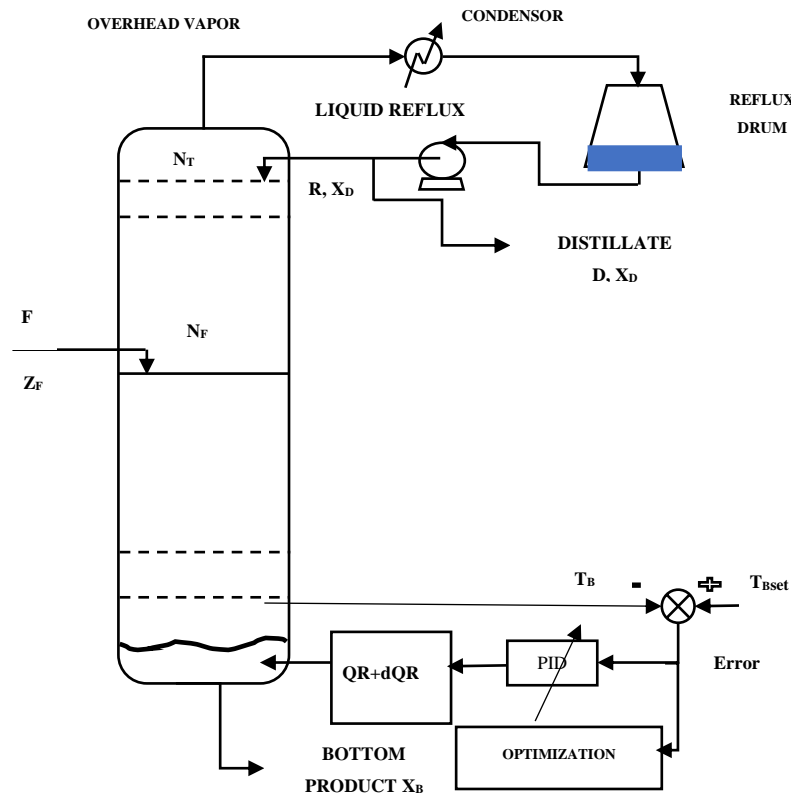


Fig. 1: Schematic diagram for distillation process

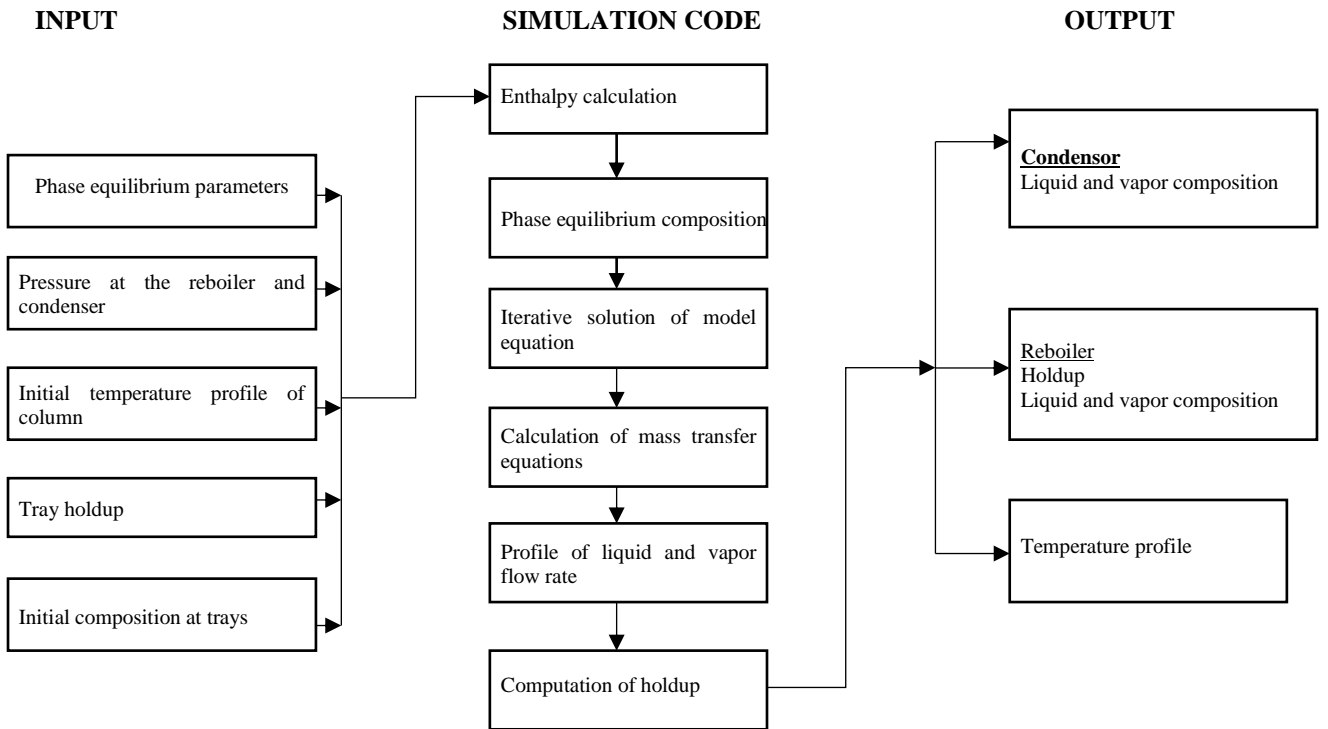


Fig. 2: Simulation chart of multicomponent distillation column

Problem formulation: The feed flow, reflux flow and reboiler heat input are the key factors which regulate the temperature profile of distillation column. Among these factors, it is essential to control the reboiler temperature because reboiler is adjacent to heat source. The main objective is to achieve the desired product quality by maintaining the reboiler temperature which is controlled by manipulating reboiler heat input. A PID controller is designed for the control purpose whose parameters are optimized using Tyreus-Luyben method, Genetic Algorithm (GA), Simulated Annealing (SA) and hybrid SAPS technique.

PID tuning Algorithms

PID Controller design: In control system design the nonlinear vector value function is denoted by $u ()$:

$$m(t)=u[t,x(t),n(t)]$$

where $m(t)$ is the manipulated variable given to the process, $x(t)$ is the state vector and $n(t)$ is the reference input. The main task of a controller is to select the feedback control law u in such a way that whole closed loop system becomes stable. The following form of PID controller for parameter u is used.

$$m(t)=k_p e(t)+k_i \int e(t) dt+k_d \frac{de(t)}{dt}$$

PID tuning using intelligent techniques: The basic block diagram of distillation process with intelligently tuned PID controller is shown in figure 3. The optimal values of PID parameters can be obtained by optimizing objective functions using different optimization techniques available in literature. In the present work genetic algorithm, simulated annealing and hybrid simulated annealing-pattern search (SAPS) are used for the purpose. The optimization problem considered is single-objective. The various optimization techniques used are discussed below.

Simulated Annealing (SA): Simulated annealing is used extensively in control system design during last few decades. Mechanics of solid annealing process marks the beginning of SA. It was first applied on combinatorial optimization problems by Kirkpatrick et al.⁹ The metropolis algorithm

simulates this process in a way the solid melts with increase in temperature accompanied by slow cooling so that solid crystallizes into minimum free energy state. Mathematically SA is a randomization device that allows wrong way movements during the search for optimum through an adaptive acceptance-rejection criterion which can treat non-convex problems efficiently. The basic SA algorithm is explained below.

Step 1: Produce enough solutions J as preliminary state. Calculate the value of the fitness function $L (J)$.

Step 2: Choose a value of the initial temperature $T_1>0$ $T_1>13$, Set iteration counter $w = 1$ $w=1$

Step 3: Repeat the following steps H times (time length):

- > In a vicinity of current state J , generate a new solution J' . Calculate fitness function $L (J')$.
- > Let $\Delta L=L(J')-L(J)$
- > If $L<0$, $J = J'$ (downward shift)
- > If $L \geq 0$, $J = J'$ with probability of $e^{\frac{-\Delta L}{T_w}}$ (upward shift)

Step 4: If a given stop condition is satisfied, stop. Otherwise, $T_{w+1} = f (T_w)$ and $w=w+1$ and go to step 3 (T_w and f denote the temperature at the w^{th} epoch and the cooling function, respectively).

Genetic Algorithm (GA): Genetic algorithm was first proposed by John Holland in 1975. It begins with an initial population having number of chromosomes where each corresponds to a solution of the given problem. The steps for implementing the GA are as follows:

- a) Generate the preliminary inhabitants of chromosomes of fixed size where each chromosome represents the probable solution.
- b) Estimate the fitness of every chromosome in the population.

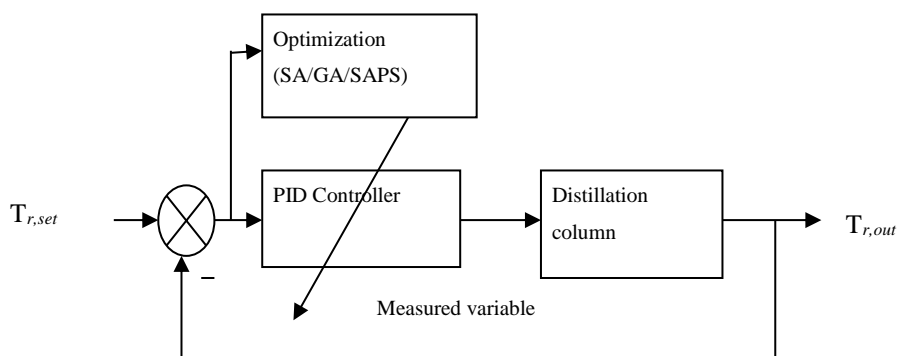


Fig. 3: The schematic diagram of distillation process control

- c) Choose the fittest element of the population.
- d) Replicate using a probabilistic method.
- e) Execute crossover operation on the reproduced chromosomes.
- f) Apply mutation operator.
- g) Reiterate from step b until a predefined convergence condition is met.

Hybrid Simulated Annealing and Pattern Search (SAPS): Simulated annealing (SA) is extensively used for solving continuous global optimization problems. It works on generation of test point in a vicinity of the present iterate and decides whether the present point should be replaced by the test point on comparison of function values. Conjunction to an optimal solution can theoretically be assured only after an infinite number of iterations controlled by the method called cooling schedule. An appropriate cooling schedule is needed in the finite-time implementation to simulate the asymptotic conjunction behavior of SA.

Because of this reason, SA suffers from sluggish conjunction rate and it may stroll around the optimal solution if high precision is requisite. To overcome this problem, hybrid function of SA and PS is used.

Simulated annealing can be combined with Pattern Search approach in two ways; first the PS approach is used to provide fine initial solution which is further improved by SA and in second approach, the simulated annealing provides a fine initial solution as a preliminary point to the alternative approach.^{1,2,17} In this study, the second approach is considered in which SA and PS are integrated to optimize the objective function to obtain the global optimum solution. A hybrid function is an optimization function that runs when global optimization terminates in order to improve the value of fitness function.

Initially the global simulated annealing will optimize the parameters and then pattern search locally optimizes these parameters i.e. the final point of SA becomes the initial point for PS. Steps for implementation of SAPS are as follows:

1. Initialization: Initial solution is obtained by using simulated annealing as discussed in step 1 to 4. When simulated annealing reaches to its optimal region then optimization will shift to basic pattern search algorithm which is based on search and poll steps to further improve the parameters value.

2. Pattern search: The final solution obtained from simulated annealing is initial solution for pattern search (obtained from SA) $c^{(0)} \in \Omega$ (obtained from SA) and an initial mesh size $\Delta_0 > 0$. Set the iteration counter $m = 0$

3. Search step: Evaluate fitness function f at a finite number of points in the mesh I_m . If $I(n) < I(c^{(m)})$ for some $n \in I_m$, then set $c^{(m+1)} = n$ and go to step 5 (the search step is deemed successful). If the search step is unproductive i.e. $f(c^{(m)}) \leq f(n)$, for all \bar{v} points in I_m then go to step 6.

4. Poll step: This step is executed only if the search step is unsuccessful.

- If $f(k_i) < f(c^{(m)})$ for some k_i in the poll set K_m , then set $c^{(m+1)} = k_i$ and go to step 5 in order to increase the mesh size Δ_m , (poll step is declared successful).

- Otherwise if $f(c^{(m)}) \leq f(k_i)$ for all k_i in the poll set K_m , set $c^{(m+1)} = c^{(m)}$ and go to step 6 in order to decrease the mesh size Δ_m , (poll step is declared unsuccessful).

5. Mesh expansion: Let $\Delta_{m+1} = \phi_m \Delta_m$, (with $\phi_m > 1$). Increase $m = m+1$ and go to step 3 for a new iteration

6. Mesh reduction: Let $\Delta_{m+1} = \theta_m \Delta_m$ (with $0 < \theta_m < 1$). Increase $m = m+1$ and go to step 3 for a new iteration.³ This function will continue till the stopping criterion is met. After execution of SAPS, final optimized values of variables are obtained on which the performance of process will be evaluated. Figure 4 shows the flowchart for implementation of SAPS tuned PID controller.

The main step in application of SAPS is to select the objective function. Various objective functions are used for optimization in the recent past and most popular ones are stated below:⁷

Integration of absolute error

$$S_1 = \int_0^{\infty} |e(t)| dt$$

Integral square error

$$S_2 = \int_0^{\infty} e^2(t) dt$$

Integration of time weighted error squared:

$$S_3 = \int_0^{\infty} t e^2(t) dt$$

where $e(t)$ is the error given by the equation:

$$e(t) = T_{Bset} - T_B$$

where T_B is the reboiler temperature to be is controlled which depends on reboiler heat input Q_R . Q_R Lies in the range $4Btu < Q_R < 6Btu$. The PID parameters are optimized by considering these objective functions using SAPS.

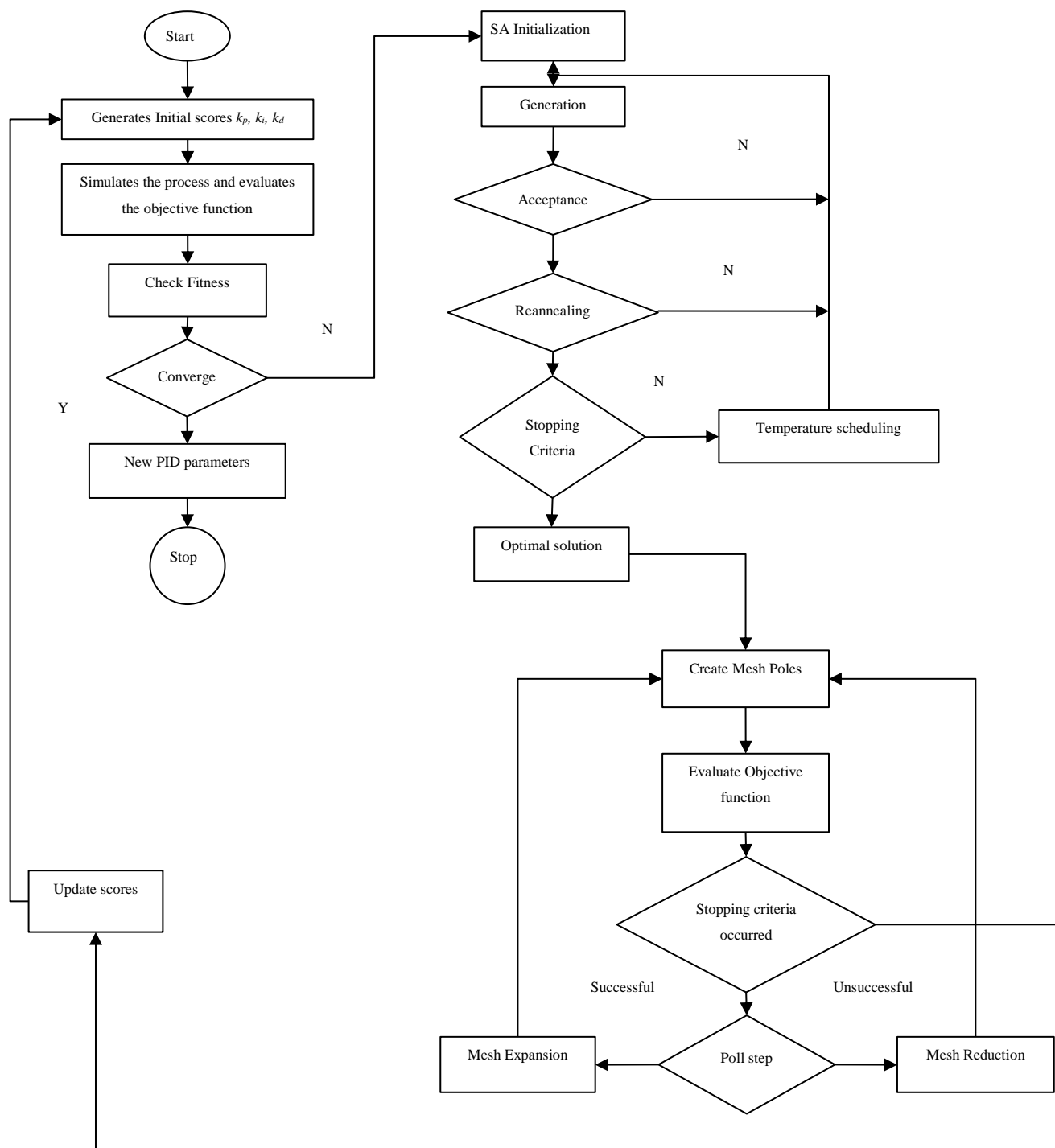


Fig. 4: Flow chart for Hybrid Simulated Annealing and Pattern Search tuning of PID controller

Results and Discussion

The mathematical model of multicomponent distillation column discussed previously is simulated in MATLAB 8.0.1.604 on PC. The task is to maintain the desired product quality by controlling the reboiler temperature. The reboiler temperature maintains the temperature profile of the process which in turn decides the product composition. The temperature profile of the process can also be controlled by controlling the reflux and temperature of different trays. Here reboiler temperature is the key factor because it is nearest to heat source and controls the whole temperature profile of distillation process.

In the present work temperature profile of distillation column is maintained by regulating the reboiler heat input as shown in figure 1. Initially conventional Tyreus-Luyben (TL) tuned PID (TL-PID) controller is designed to achieve the control objective. The values of PID parameters obtained from Tyres-Luyben (TL) are shown in table 1. The reboiler temperature achieved with the help of TL-PID is shown in figures 5(a) and the corresponding composition variations are given in figure 5(b)-5(e). The composition XD3, XD4, XD5 in distillate and XB1, XB2, XB3 in bottom product is negligible and therefore not shown in the results.

The set point for the reboiler temperature is considered as 202 °F. It is observed from the above results that TL-PID controller provides large settling time and rise time with some offset error. Hence the performance of TL-PID is not satisfactory in transient as well as steady state. Moreover, as discussed previously Tyreus-Luyben (TL) tuning method executes well for lower order processes but gives average performance for higher order and non-linear systems.

In order to achieve the better performance, fast response of the system and to overcome the problems of conventional tuning method, intelligent tuning methods discussed previously i.e. GA and SA are used for the design of PID controller leading to GA-PID and SA-PID controllers

respectively. The PID parameters for the two controllers are given in table 1. The results obtained using GA-PID and SA-PID controllers are shown in figure 6.

It is observed from figure 6 that the reboiler temperature reaches the steady state earlier in case of GA-PID and SA-PID as compared to TL-PID. This is due to the reason that optimized PID parameters are used in the controller and perform efficiently. It is also observed that in case of GA-PID and SA-PID the steady state error and settling time, both are reduced with improved rise time. It is also observed from the results that SA optimization is better in comparison to GA. Hence due to better control of reboiler temperature, the product quality is also improved.

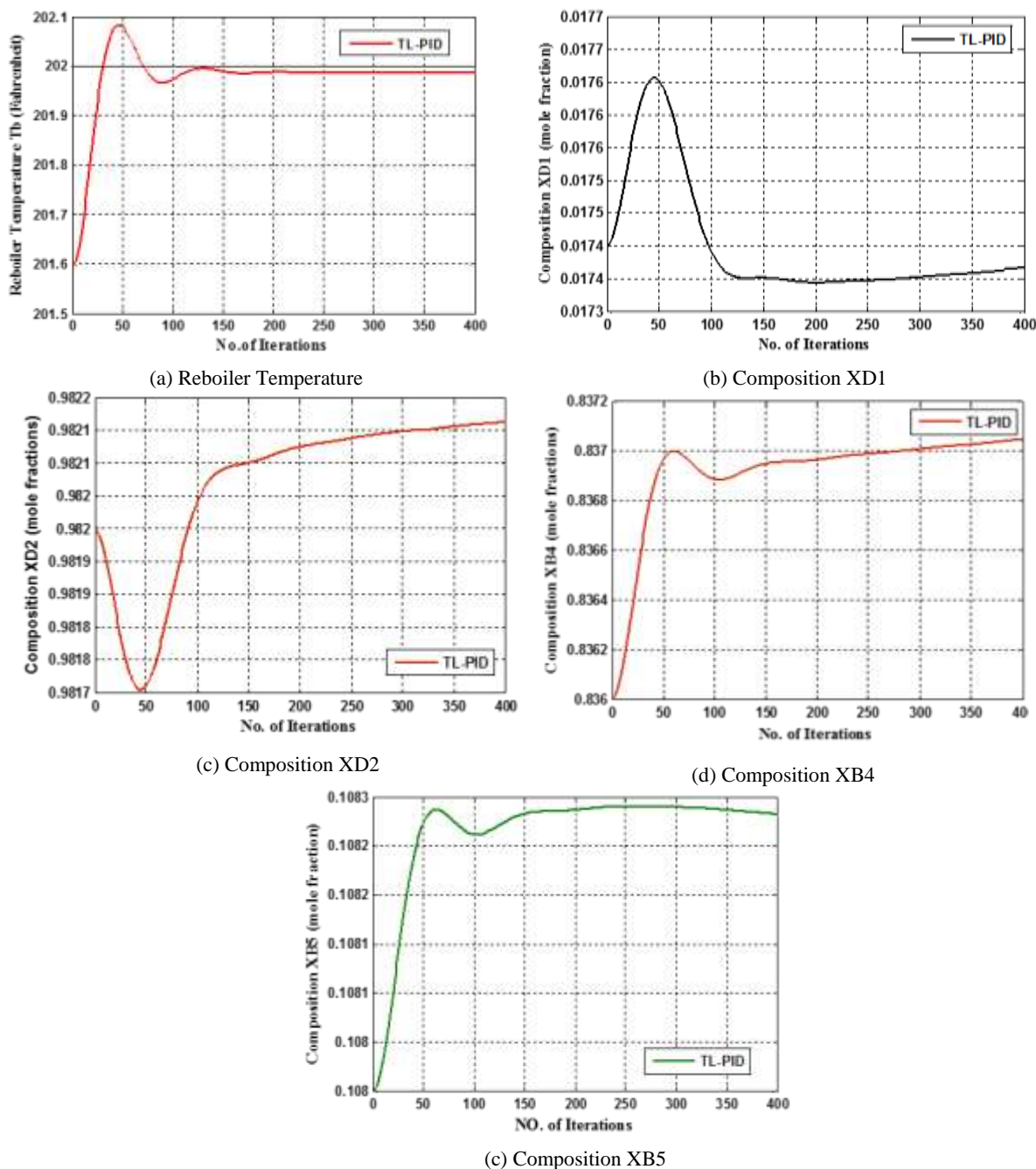
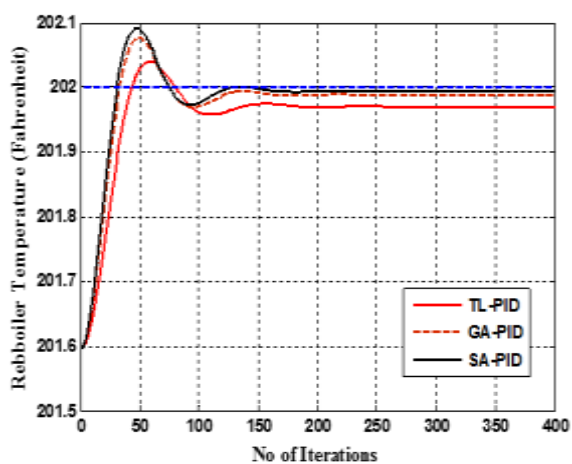
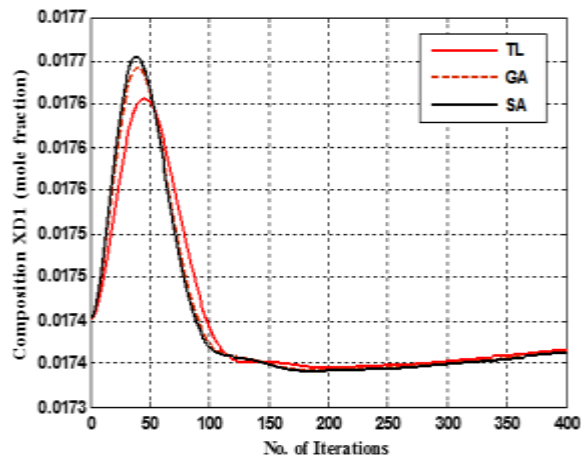


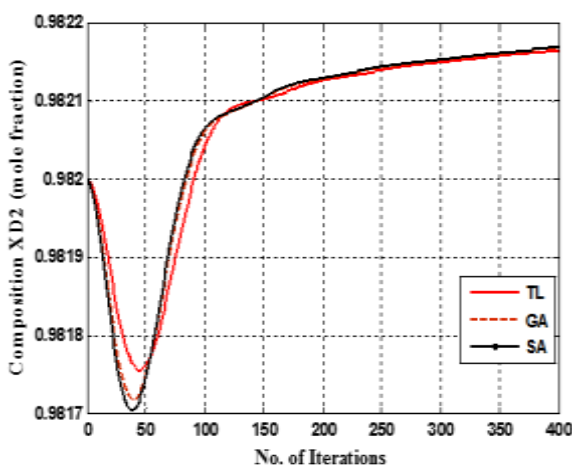
Figure 5: Re-boiler temperature and corresponding composition variations



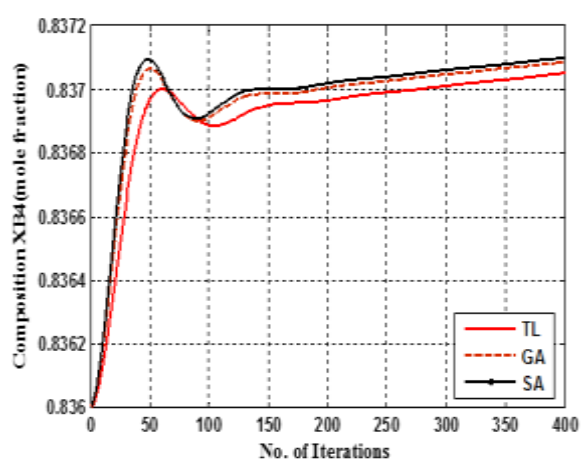
(a) Reboiler Temperature



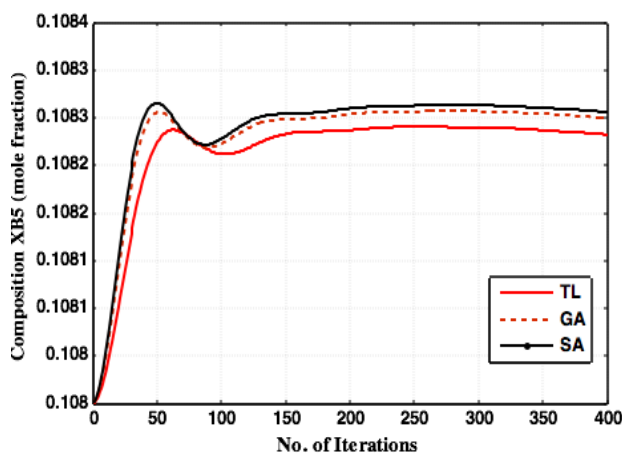
(b) Component XD1



(c) Component XD2



(d) Component XB4



(e) Composition XB5

Fig. 6: The Reboiler temperature and product compositions for TL-PID, GA-PID and SA-PID controller

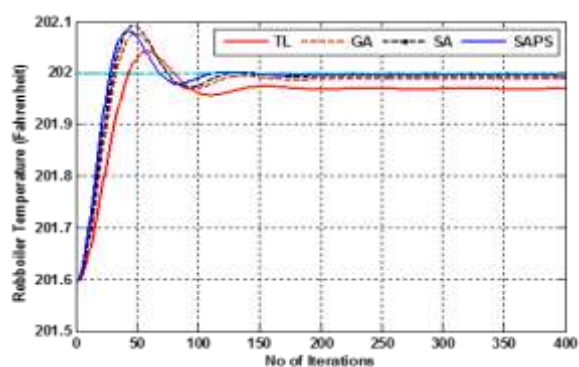
Table 1
Parameter of tuned PID with T-L, SA and GA

Tuning methods	Kp	Ki	Kd
TL	0.0523	0.000242	0.8131
SA	0.0835	0.000108	0.9132
GA	0.0762	0.000184	0.9062

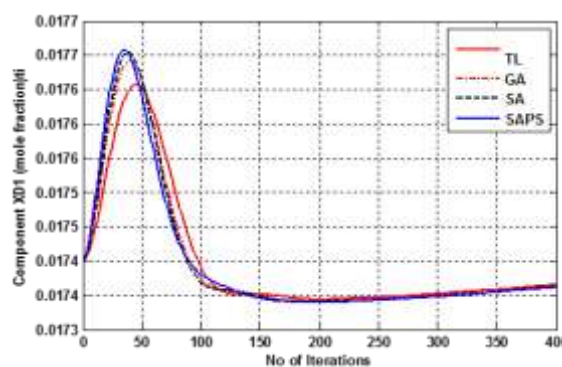
As the GA-PID and SA-PID are more efficient and effective as compared to TL-PID, appropriate cooling schedule is needed in the finite-time implementation to simulate the asymptotic conjunction behavior of SA. Because of this reason, SA suffers from sluggish conjunction rate and it may stroll around the optimal solution if high precision is requisite. Further GA takes more time to converge to the optimal solution which makes it very slow. Therefore, to overcome the problem of SA and GA, a local search method i.e. Pattern search is hybrid with simulated annealing to form the SAPS search algorithm. Initial scores for simulated annealing are provided by using Tyreus-Luyben method. As discussed previously, three objective functions are optimized to evaluate the PID parameters using SAPS. The optimized PID parameters for three objective functions and corresponding quantitative analysis are given in table 2. It is

observed from the table that objective function S_1 gives the best rise time, settling time and an acceptable overshoot, therefore objective function S_1 is used to obtain the optimum PID parameters.

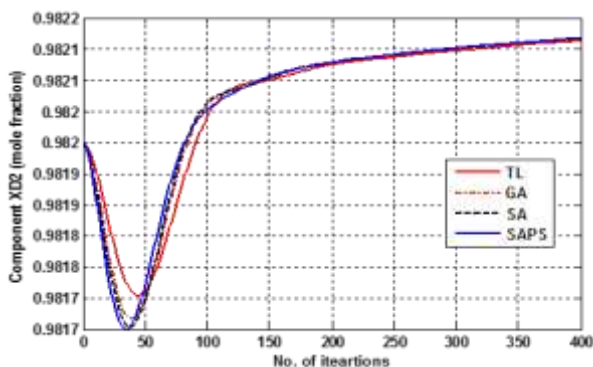
The performance comparison of all the designed controllers is shown in figure 7. It is observed from the results that reboiler temperature reaches steady state after 96 iterations for SAPS-PID controller whereas for GA-PID, SA-PID and TL-PID take 116, 110 and 124 iterations respectively. The quantitative analysis is summarized in table 3. SAPS-PID not only takes lesser time to settle but also rise time and mean square error (MSE) at steady state are better in comparison to other techniques. The designed controllers are tested for set point tracking and disturbance rejection.



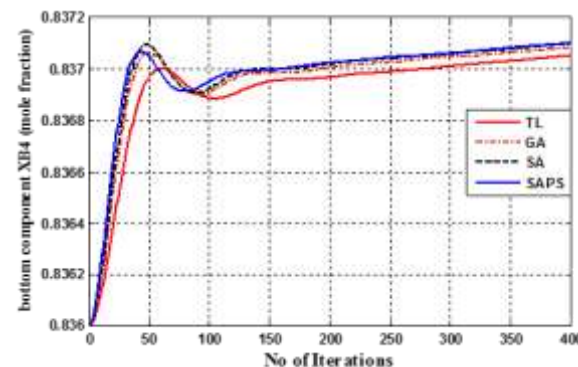
(a). Reboiler temperature



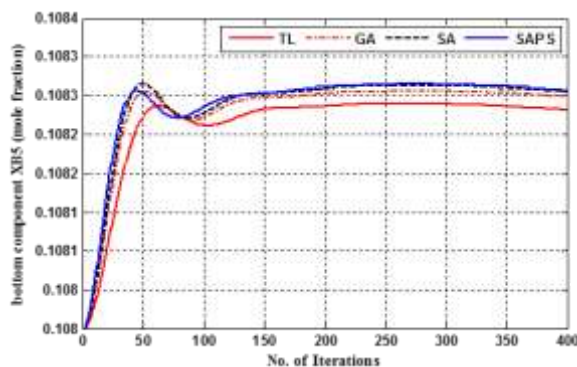
(b). Component XD1



(c). Component XD2



(d). Composition XB4

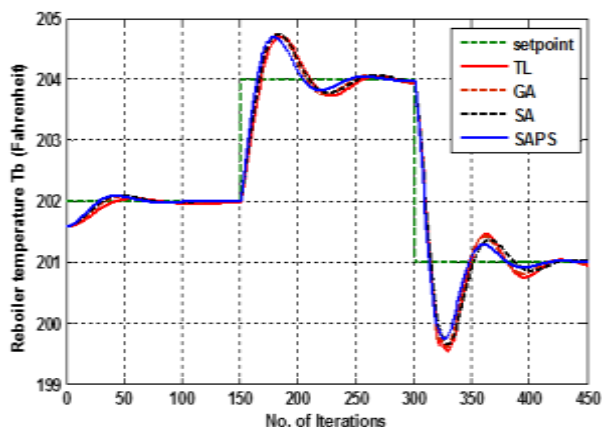


(e). Composition XB5

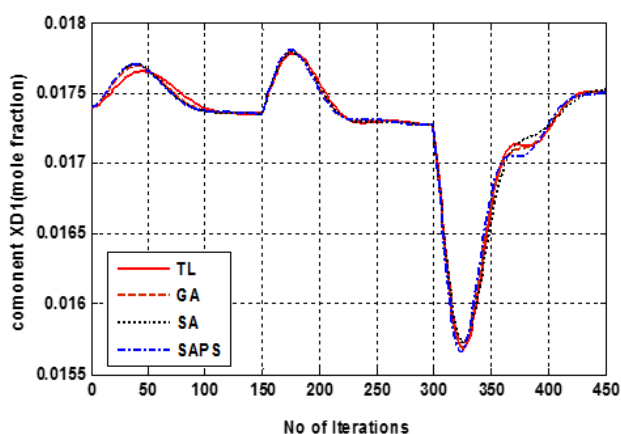
Fig. 7: Comparison of all the controllers TL-PID, GA-PID, SA-PID, SAPS-PID

Set point tracking: The robustness of the controller is verified by observing its adaptation to the changes in operating conditions. Two types of changes are incorporated in the set point i.e. positive and negative change. The experimental analysis reveals that the set point of reboiler temperature can be varied from 200°F to 212°F. If the set point is beyond this range, the distillate quality is degraded. Hence the set point for reboiler temperature is changed from 202°F to 204°F for positive at 150th iteration and from 204°F to 201°F for negative change at 300th iteration.

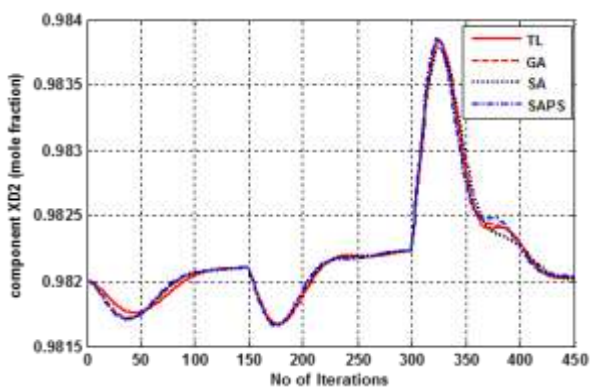
The responses obtained for positive and negative set point changes are shown in fig. 8 (a). It is observed from the results that SAPS-PID adapts the change in the operating point more efficiently as compared to other designed controllers. The mean square error for different controllers is summarized in table 4 which again proves the robustness of SAPS-PID as compared to other designed controllers. It is observed from figure 8 that change in the set point of reboiler temperature affects the composition of distillate and bottom product accordingly.



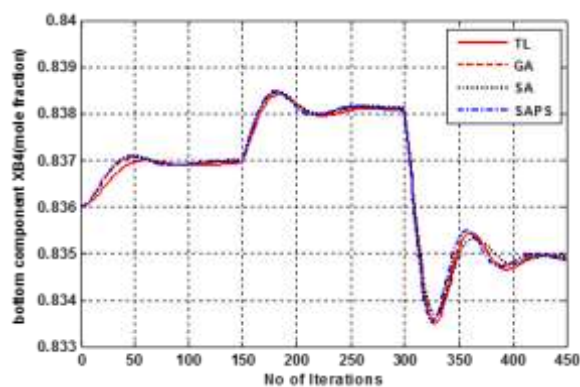
(a) Positive and Negative change in temperature



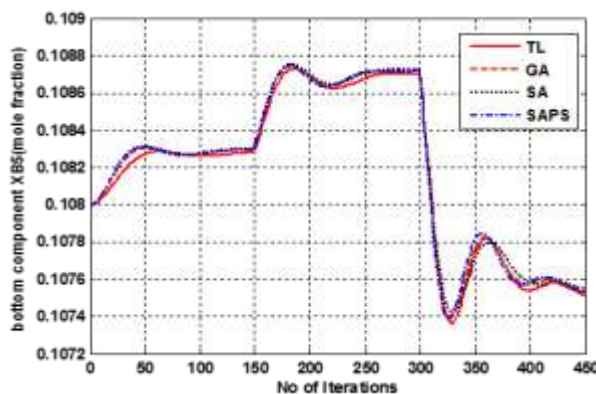
(b) Composition of XD1



(c) Composition of XD2



(d) Composition of XB4



(e) Composition of XB5

Fig. 8: Effect of positive and negative change in Reboiler temperature, different compositions

Table 2
Comparison of different objective functions

Objective Function	K_p	K_i 10^{-4}	K_d	T_r	T_s	%OS
S ₁	0.1050	2.00	1.15	18	96	0.0431
S ₂	0.084	2.10	0.92	20	133	0.0417
S ₃	0.086	2.40	0.91	21	134	0.0481

Table 3
Performance indices for different techniques

Controller	T_r	T_s	% os
TL-PID	26	124	0.0351
GA-PID	20	110	0.0428
SA-PID	20	109	0.0485
SAPS-PID	18	96	0.0431

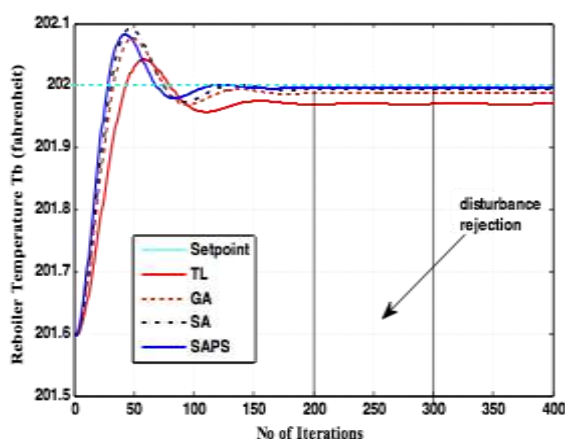


Fig. 9: Reboiler temperature for -10% disturbances in feed

Table 4
Mean square error (MSE) of controller

Controller	Temperature control (MSE)	Set point tracking (MSE)	MSE (-10% disturbance)
TL-PID	0.00769	1.4908e-002	0.008124
GA-PID	0.00598	1.2665e-002	0.006427
SA-PID	0.00573	1.2390e-002	0.006175
SAPS-PID	0.00468	1.0178e-002	0.00417

Conclusion

The research work focuses on precise control of product composition which is attained by controlling the reboiler temperature. A hybrid simulated annealing and pattern search based PID controller is designed for the purpose. The comparative analysis of the proposed controller is carried out by comparing the performance with GA-PID, SA-PID and conventional PID controllers. It is observed from the results that SAPS-PID not only takes lesser time to settle but also its rise time and mean square error are lesser as compared to other techniques. The designed controllers are also tested for set point tracking and disturbance rejection which verifies the robustness of proposed hybrid controller. Hence it is concluded that hybrid SAPS-PID controller may prove to be a better controller for nonlinear and complex processes.

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