DYNAMIC OPTIMIZATION OF ACETYLENE HYDROGENATION UNIT USING A HYBRID GA-SQP ALGORITHM

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Abstract

Dynamic simulation and dynamic optimization of an industrial hydrogenation reactor system were developed and investigated in the present work. The process consists mainly of three adiabatic fixed bed hydrogenation reactors in series in addition to one heater before the first reactor and three coolers after each reactor for interstage cooling. The feed flow rate to the unit, the feed temperature or the carbon monoxide content of the feed may change and causes variations of the outlet temperature of reactors. Therefore, it is essential to control the inlet temperature of each reactor. There is a temperature controller before each reactor and also one after the third reactor. The tuning parameters of the controllers were optimized dynamically in three different cases, taking into account the process constraints and catalyst deactivation. In each case, a special disturbance is forced to the process. Optimization of the process was done by the use of a hybrid GA-SQP method. The new hybrid method was developed to overcome the difficulties of both methods. The genetic algorithm (GA) which is a stochastic method, is relatively slow, but is not sensitive to the initial point. In contrast, sequential quadratic programming (SQP) method is a deterministic method which is fast, but very sensitive to the starting point and gets trapped in local optima. In the newly developed hybrid method, the SQP method speeds the solving procedure, while the GA enables the algorithm to escape from local optima. An industrial acetylene hydrogenation system is used to provide the necessary data to adjust kinetics and to validate the approach.

Keywords: Hydrogenation, Dynamic optimization, Process control

Presenting Author's biography

Navid Mostoufi is an Associate Professor of Chemical Engineering at the University of Tehran. His research interests are in the fields of multiphase reactors, process modeling and optimization and numerical methods. He holds a B.Eng. and M.S. degrees in Chemical Engineering from the University of Tehran, Iran, plus a Ph.D. in Fluidization from Ecole Polytechnique de Montreal, Canada. He is the co-author of the textbook Numerical Methods for Chemical Engineers with MATLAB Application, published by Prentice Hall PTR in 1999. He is also editor of the journal of Chemical Product and Process Modeling, published by Berkeley Electronic Press (www.bepress.com/cppm).

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1 Introduction

There are various problems of dynamic optimization in chemical engineering. Dynamic optimization of batch reactors [1-3] is one of these problems. Another category is determining the optimal flow rate for a plant or inlet temperature profile of reactors [4]. Determination of the optimal set of some essential parameters for a special operational unit is another example of optimization problems [5].

Different methods are used in dynamic optimization. Good illustrations are numerical solutions and sequential strategies [1], genetic algorithm [2], evolutionary algorithms [3], sequential quadratic programming (SQP) [5].

Determination of optimal set of control tuning parameters is a relatively new area in dynamic optimization. Duty of a controlling system in an industrial plant is to control the essential parameters such as temperature, pressure, level and flow rates. An appropriate controlling system must be able to control disturbances rapidly. The speed of controlling system is very important in emergency situations. Moreover, it is desired to reach the steady state conditions as soon as possible in start-up of the plant. These facts show the importance of a fast and robust controlling system.

Besides the speed of controllers, another capability, which is expected from a controlling system, is to control any kind of disturbance. A controlling system should respond properly to any disturbance occurring in the plant. This is important because a controlling system may control a disturbance very fast, however, when another disturbance occurs, the controllers might case oscillation. Therefore, the set of tuning parameters of the controller should be set such that enable the controller to control any kind of disturbances.

In this work, the set of optimal control tuning parameters were determined by a newly developed optimization method. To test each controlling system, its response to typical disturbances should be studied. Thus, three common disturbances which normally occur in a real plant were used for testing the parameters.

2 Process modeling

The duty of the hydrogenation system in an olefin plant is to eliminate acetylene, propyne and propadiene, butadiene and other higher unsaturated olefins from dry cracked gas stream by converting them in a catalytic selective hydrogenation step to lower unsaturated olefins and paraffins. The hydrogenation is performed in three adiabatic fixed-bed reactors in series. The reactor design is identical for all three hydrogenation reactors. The heat of the exothermic reaction is removed against cooling water down stream of each reactor. Six reactions take place in these reactors. These reactions are shown in Tab. 1.

As shown in Fig. 1, the hydrogenation is performed in a system with multiple adiabatic fixed bed reactors (R_1, R_2, R_3) in series with coolers (E_1, E_2, E_3) after each reactor. The heat of the exothermal reactions is taken off by cooling water. Before the first reactor and also after each reactor, there is one temperature controller (TC-1, TC-2, TC-3, TC-4). The inlet temperature of the first reactor can be controlled by LP steam flow rate. The pressure of this steam flow is controlled by PC. The temperature of the cracked gas down stream of each reactor can be adjusted by bypassing the coolers. In case of a too high outlet temperature of the reactor, additionally cooling water flow to the coolers can be increased. The feed is heated by LP steam via heater (H).

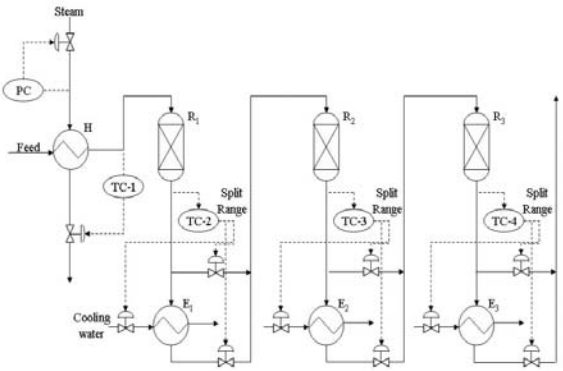

Fig. 1 Schematics of the hydrogenation system

Tab. 1 Hydrogenation reactions considered in this work

Component No.	Component Name	Hydrogenation Reaction
1	acetylene	$C_2H_2 + H_2 \rightarrow C_2H_4$
2	ethylene	$C_2H_4 + H_2 \rightarrow C_2H_6$
3	propyne	$C_3H_4 + H_2 \rightarrow C_3H_6$
4	propadiene	$C_3H_4 + H_2 \rightarrow C_3H_6$
5	1-butene 3-yne	$C_4H_4 + H_2 \rightarrow C_4H_6$
6	1,3-butadiene	$C_4H_6 + H_2 \rightarrow C_4H_8$

The rates of the reaction listed in Tab. 1 were adopted from Gobbo et al. [6]:

$$(-r_i) = \frac{k_i C_i C_H \rho_S (1-\varepsilon)}{\left[1 + (k_H C_H)^{\frac{1}{2}} + k_{CO} C_{CO}\right]^3} \qquad (1)$$

where

$$k_i = k_{0,i} \exp\left(-\frac{E_i}{RT}\right) \quad (2)$$

The catalyst becomes deactivated as the operation proceeds. The reaction rate on the deactivated catalyst could be expressed by:

$$r_{i,d} = r_i \, a(t) \quad (3)$$

Brown et al. [7] assumed that there is a uniform fouling of green oil over the length of the reactor so that there would be an average catalyst deactivation term for the entire bed. Considering that the formation of green oil is proportional to the acetylene concentration and taking into account the main deactivation equations in the literature [7, 8], the following empirical equation was proposed by Gobbo et al. [6]:

$$\frac{da}{dt} = -C_{acetylene}^{\theta} \, k_a \exp\left(\frac{-E_a}{RT}\right) \quad (4)$$

The kinetic parameters for these equations were determined by Mansoornejad [9]. Tab. 2 presents these kinetic parameters.

Tab. 2 Kinetic parameters

Parameter	Unit	Value
$k_{0,Acetylene}$	$m^6/mol.kg_{cat}.s$	1.96×10^9
$E_{Acetylene}$	J/mol	30.90
$k_{0,Ethylene}$	$m^6/mol.kg_{cat}.s$	1.02×10^7
$E_{Ethylene}$	J/mol	25.12
$k_{0,Propyne}$	$m^6/mol.kg_{cat}.s$	1.38×10^9
$E_{Propyne}$	J/mol	48.88
$k_{0,Propadiene}$	$m^6/mol.kg_{cat}.s$	2.63×10^8
$E_{Propadiene}$	J/mol	43.93
$k_{0,1,3\text{-}butadiene}$	$m^6/mol.kg_{cat}.s$	1.87×10^9
$E_{1,3\text{-}butadiene}$	J/mol	25.25
$k_{0,1\text{-}Butene\ 3\text{-}yne}$	$m^6/mol.kg_{cat}.s$	1.33×10^9
$E_{1\text{-}Butene\ 3\text{-}yne}$	J/mol	49.17
$k_{0,Hydrogen}$	mol/m^3	5.01×10^4
$E_{Hydrogen}$	J/mol	84.57
$k_{0,CO}$	mol/m^3	2.00×10^5
E_{CO}	J/mol	43.93
k_a	$m^{3\theta}/mol^{\theta}.s$	3.69×10^8
E_a	J/mol	0.389
θ	-	4.11

The inlet temperature of the first reactor and the outlet temperature of all three reactors must be controlled. Disturbances in temperature may occur because of variation in cracked gas flow rate, malfunction of propylene refrigerant system which causes the increase or decrease the inlet temperature of cracked gas to hydrogenated unit and changes in the carbon monoxide content of the feed can make some deviations in reactors temperature. All of these cases force the system to have fast and robust controllers. Considering the controllers to be Proportional – Integral (PI), according to Eq. (5), the optimum set of K_p and K_i parameters for all controllers should be found.

$$A = A_{cte} + K_P \left[e + K_i \int_0^t e(t)dt \right] \quad (5)$$

3 Optimization problem definition

Optimization techniques are used to find a set of design parameters, $x = \{x_1,\ldots,x_n\}$, of a system, that can lead the system to its optimal conditions. In a more advanced formulation, the objective function, $f(x)$, to be minimized or maximized, might be subject to constraints in the form of equality, inequality and/or parameter bounds. A general optimization problem definition could be stated as:

$$\begin{aligned} &Minimize \quad f(x) \\ &subject\ \ to \\ &G_i(x) = 0 \quad , \quad i = 1,\ldots, m_e \\ &G_i(x) \le 0 \quad , \quad i = m_e + 1,\ldots, m \end{aligned} \quad (6)$$

where x is the vector of n design parameters, $f(x)$ is the objective function, which returns a scalar value and the vector function $G(x)$ returns a vector of length m containing the values of the equality and inequality constraints evaluated at x. Design parameters, x_i, are the decision or control variables by changing which the optimum point of the objective function could be found.

In the present work, the controller tuning parameters were determined by optimization. This objective function must show the effect of controlling time and error simultaneously. The difference between set point and process value divided by set point in each controller was considered as the error. The duration in which the error becomes zero was considered as the controlling time. Thus, the objective function in this work was defined as the integral of the product of time and error.

$$f = \int_0^{t_f} e(t)dt \quad (7)$$

where the error is

$$e = \left| \frac{SP - PV}{SP} \right| \quad (8)$$

The optimization technique was used to determine the decision variables, i.e., the controller tuning parameters,

so that the objective function given in Eq. (7) would be minimized.

4 Genetic algorithm (GA)

The GA is a stochastic method for solving both constrained and unconstrained optimization problems and is based on natural selection, the process that drives biological evolution. This algorithm could be applied to solve a variety of optimization problems that are not well suited for standard optimization algorithms, including problems in which the objective function is discontinuous, nondifferentiable, stochastic, or highly nonlinear. The GA starts with an initial random population which presents the first generation. Each population consists of some individuals and each individual is made of a number of genes. These genes are decision or control variables. The objective function is calculated for each individual on the basis of its genes. Populations will be repeatedly modified to reach the solution which would be the best individual. At each step, the GA selects the individuals from the current population on the basis of their scores to represent the parents and uses them to produce children or the next generation. Over successive generations, the population evolves towards an optimal solution.

4.1 Termination criteria

The GA creates generations by selecting and reproducing parents until a termination criterion is met. One of the stopping criterions is a specified maximum number of generations. Another termination strategy involves population convergence criteria. In general, the GA forces the majority the population to converge to a single solution. When the sum of the deviations among individuals becomes smaller than some specified threshold, the algorithm could be terminated. The algorithm could also be terminated due to a lack of improvement in the best solution over a specified number of generations.

5 Sequential quadratic programming (SQP)

The SQP methods are appropriate for solving smooth nonlinear optimization problems when the problem is not too large, functions and gradients can be evaluated with sufficiently high precision and the problem is smooth and well-scaled (Hock and Schittkowski, [10]). Consider the general form of an optimization problem, such as the one shown in Eq. (6). All the functions, including the objective function $f(x)$ and constraints $G(x)$, must be continuously differentiable. The solution procedure is on the basis of formulating and solving a quadratic sub-problem in each iteration. The sub-problem is obtained by linearizing the constraints and approximating the quadratic Lagrangian function [10]:

$$L(x,\lambda) = f(x) + \sum_{i=1}^{m} \lambda_i G_i(x) \tag{9}$$

At each iteration, an approximation is made of the Hessian of the Lagrangian function using a quasi-Newton updating method [10].

The process would be proceeded from given iteration x_k, which is an approximation of the solution, λ_k an approximation of the multiplier and H_k which is an approximation of the Hessian of the Lagrangian function. Then, the following quadratic programming (QP) sub-problem is formed to solve:

$$\begin{aligned} &Minimize \quad \frac{1}{2} d^T H_k d + \nabla f(x_k)^T d \\ &\nabla G_i(x_k)^T d + G_i(x_k) = 0 \quad , \quad i = 1,...,m_e \\ &\nabla G_i(x_k)^T d + G_i(x_k) \geq 0 \quad , \quad i = m_e+1,...,m \\ &d \in R^n \end{aligned} \tag{10}$$

The matrix H_k is a positive definite approximation of the Hessian matrix of the Lagrangian function. This sub-problem is a QP sub-problem whose solution is used to form a search direction d_k for a line search procedure. In other words, the solution is used to form the next iterate:

$$x_{k+1} = x_k + \alpha_k d_k \tag{11}$$

The step length parameter α_k is determined by an appropriate line search procedure so that a sufficient decrease in a merit function is obtained. The merit function of the following form is used in this implementation:

$$\psi(x) = f(x) + \sum_{i=1}^{m_e} \upsilon_i G_i(x) + \sum_{i=m_e+1}^{m} \upsilon_i \max\{0, G_i(x)\} \tag{12}$$

where υ_i is the penalty parameter which is initially set to

$$\upsilon_i = \left\| \frac{f(x)}{G_i(x)} \right\| \tag{13}$$

This ensures larger contributions to the penalty parameter from constraints with smaller gradients which would be the case for active constraints at the solution point.

6 Hybrid GA-SQP

The problem of determination of control tuning parameters has lots of local optima. Deterministic methods would get trapped in these local minimum. On the other hand, GA converges to the solution very

slowly, especially in final generations in which the objective function is very close to the optimal solution. Nevertheless, deterministic methods such as SQP would lead to the final solution very fast, if there is a good initial point. Thus, it could be proposed to combine these two methods in which GA is applied first to produce the proper starting point after which the calculations would shift to SQP. In other words, GA and SQP would be used in series.

Jang et al. [11] combined GA and quadratic search in parallel for optimization. When becoming close to a local minimum, it takes time for the GA to escape from this local minimum. Jang et al. [11] tried to reduce the time required for the GA to escape from the local minima by using the quadratic search in these situations. In each GA population, an additional individual would be made by the quadratic search using individuals close to the local optimum. Therefore, both GA and quadratic search would be used in parallel to make optimal individuals. Of course, the problem would be solved by the GA and quadratic search is used only to create an individual near the optimum point.

Initially, it might be proposed to use the same idea and combine the GA and SQP in parallel (i.e., applying the faster SQP method when the GA is not able to escape from the local minimum) in order to speed up the calculations and reach the final solution with fewer function evaluations. However, we found that using GA and SQP in parallel does not necessarily make the calculations faster since the gradient becomes very small in the local optima zones [9]. This drawback could be attributed to the large number of decision variables in this work (10 decision variables in this work compared to 4 in Jang et al. [11]). As discussed by Jang et al. [11], when the size of the cluster of individuals is small enough, the space corresponding to the cluster could be estimated by a quadratic model and the solution obtained by the quadratic search would be very close to the optimum for a continuous objective function. In the present work, however, the objective function is not smooth and also the gradients are very small when close to the local optima which make this method very slow. In fact, it could be demonstrated that it takes longer for SQP than GA to find the local optima in the problem of this work [9].

Based on the above discussion, a new hybrid algorithm was proposed in this work which uses the GA and the SQP in series. The algorithm starts with the GA since the SQP is not sensitive to the starting point. The calculation continues with the GA for a specific number of generations (defined by the user) during which the approximate solution becomes close to the final solution. The algorithm then shifts to the SQP which is a faster method. If the step size of the SQP is not large enough to proceed, the algorithm will shift to the GA again. Otherwise, it continues until no improvement in the objective function is observed. This sequence of shifting between GA and SQP in series could be applied more than once until the final solution is reached. Details of this procedure are illustrated in the flowchart shown in Fig. 2.

7 Results and Discussion

The set of industrial hydrogenation reactors and heat exchanger network were simulated on INDISS (Ver. 1.5.3) platform. The operating conditions and the specification of the inlet and outlet flow of each reactor are given in Tab. 3. It is worth noting that the middle of run (MOR) is 10 months and the end of run (EOR) is 24 months after the start of run (SOR). Because of catalyst deactivation, reaction rates decrease during the process. Therefore, the inlet temperature of each reactor has to be increased with time in order to compensate the reduction in reaction rates.

Tab. 3 Operating conditions of the hydrogenation reactors

Parameter	Unit	Reactor 1		Reactor 2		Reactor 3	
		In	Out	In	Out	In	Out
Temp.							
SOR	ºC	55	75.1	55	70.2	55	59.7
MOR	ºC	72.5	92.5	72.5	87.6	72.5	76.9
EOR	ºC	90	110	90	105	90	94.7
Pres.	bar(a)	35.4	34.6	34.4	33.7	33.5	32.7
H_2	mole %	29.5	29	29	28.7	28.7	28.6
C_2H_2	mole %	0.2	0.1	0.1	0.05	0.05	0
C_2H_4	mole %	32.3	32.6	32.6	32.8	32.8	32.9
C_2H_6	mole %	16.1	16.4	16.4	16.6	16.6	16.5
C_3H_4	mole %	0.13	0.1	0.1	0.06	0.06	0.04
C_3H_6	mole %	3.8	3.9	3.9	4.05	4.05	4.1
C_4H_4	mole %	0.02	0.01	0.01	0	0	0
C_4H_6	mole %	0.85	0.42	0.42	0.17	0.17	0.01
C_4H_8	mole %	0.45	0.89	0.89	1.16	1.16	13.3

The data were gathered from the hydrogenation unit of Marun Petrochemical Plant (south of Iran) at start of the run, middle of the run and end of the run of the reactors so that catalyst deactivation could be also investigated by these data. The INDISS simulation platform was then linked to MATLAB which would perform the optimization by the algorithms described above. At each iteration, the temperature data obtained from the simulator were used by the optimization program for evaluating the objective function. The program was written in such a way that if the controlling system can not control the disturbances after 20 minutes, it would stop and a new set of parameters would be applied. This procedure continues until the sum of deviations between process values and set points become lower than the specified value.

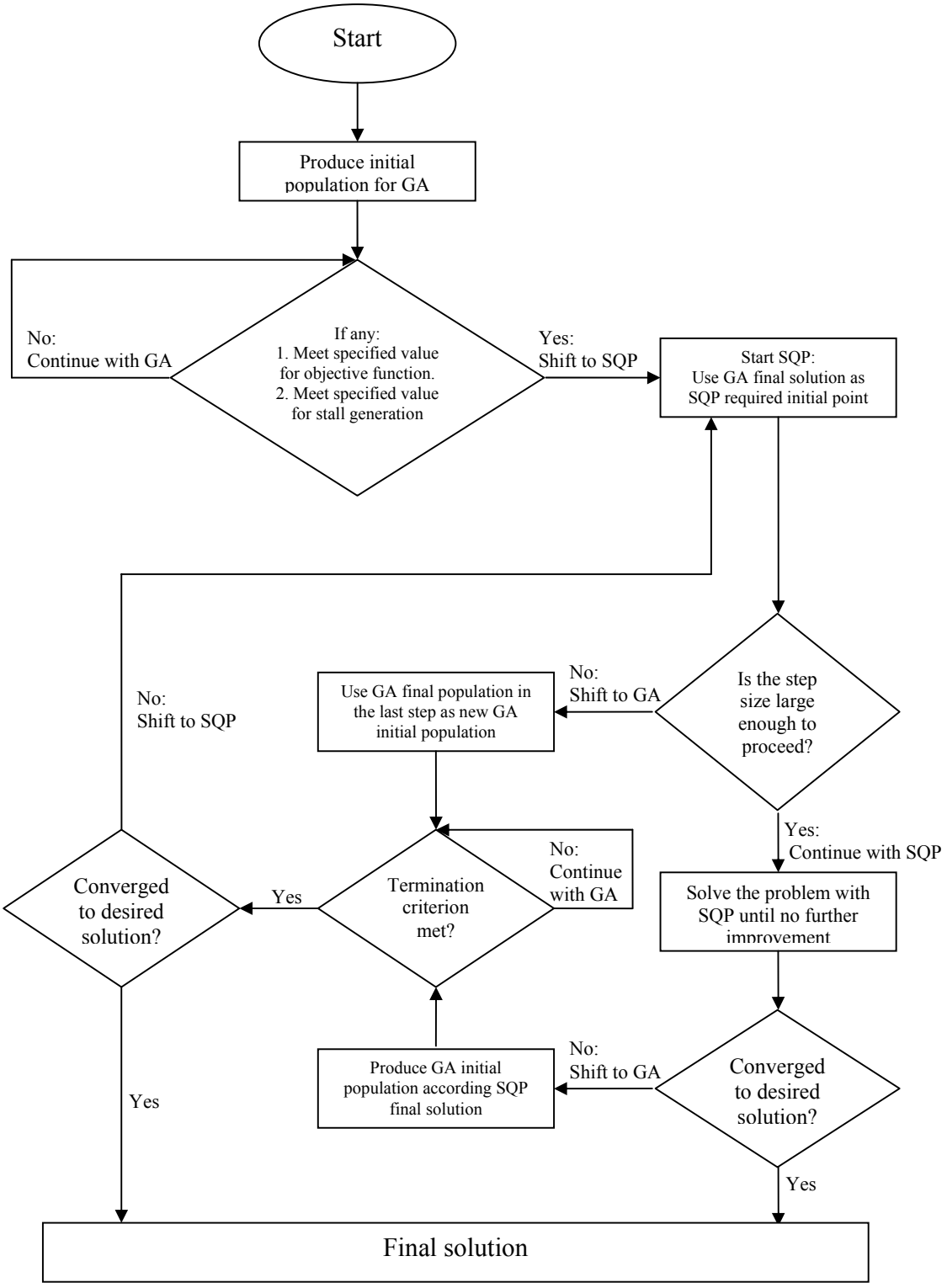

Fig. 2 Flowchart of the GA-SQP hybrid algorithm

Lower and upper bounds of the parameters are given in Tab. 4. There are some inequality constraints for temperature due to the temperature alarms which are applied for the outlet temperature of each reactor in plant. These constraints are presented in the Tab. 5.

Tab. 4 Lower and upper bounds of the parameters

Parameter	Lower bound	Upper bound
K_P	0	10
Ki	0	10
T	55	90

Tab. 5 Inequality constraints

Unit operation	Constraint (°C)
1st reactor	$T_{OUT} \leq 140$
2nd reactor	$T_{OUT} \leq 130$
3rd reactor	$T_{OUT} \leq 120$

7.1 Determination of control tuning parameters

The problem was solved for three cases. In each case, a disturbance was imposed to the system. Disturbances were selected according to the typical disturbances which could happen in the real plant. The disturbances are listed below:

- 10% change in feed temperature
- 10% change in feed flow rate
- 100% change in CO mole fraction

7.1.1 Change in feed temperature

In the first case, it was assumed that the inlet temperature of the first reactor would be reduced by 10%. The control tuning parameters derived from hybrid algorithm are presented in Tab. 6. Moreover, the variations of temperatures which are controlled are shown in the Fig. 3. The disturbance occurred in the inlet of the system, so it influences most on the first controllers. As the first controller controls the disturbance, it does not affect the next controllers.

Tab. 6 Parameters derived from GA-SQP for the first disturbance

Controller	K_P	unit	Ki	unit
PIC	1.984	1/bar	2.385	s^{-1}
TIC-1	1.785	1/°C	27.547	s^{-1}
TIC-2	0.398	1/°C	5.329	s^{-1}
TIC-3	0.412	1/°C	1.753	s^{-1}
TIC-4	0.418	1/°C	1.497	s^{-1}

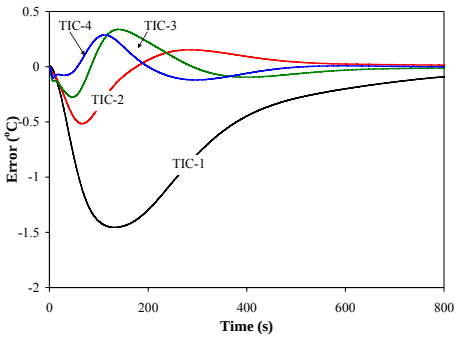

Fig. 3 Temperature deviations vs. time for first disturbance

This problem was solved by the GA and the SQP, separately and then by the hybrid GA-SQP method.

SQP is not an appropriate algorithm for solving the problem. The results of solving the problem with the SQP using different initial points are shown in Tab. 7. By comparing the objective function value at the first and final iterations, it could be seen that almost no improvement has happened and the algorithm has been trapped in the local optima in all trials.

Tab. 7 Result of solving the problem with the SQP

Initial Point	Function evaluation	Objective function value in the first iteration	Final value of objective function
Upper Bound	69	1.951	1.944
Lower Bound	63	1.989	1.983
Middle Point	91	1.903	1.847
Same as GA	107	1.917	1.830

The results of solving the problem with the GA and hybrid GA-SQP are presented in Tab. 8.

Tab. 8 Number of objective function evaluations in the GA and GA-SQP

Algorithm	No. of function evaluations	Best f
GA	2460	0.9170
GA-SQP	1192	0.9166

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It can be observed that the required number of objective function evaluations for the hybrid algorithm is less than the half of that for the GA alone. As it was mentioned before, in this part the duration in which the program runs is not constant, however, each trial takes between 40 to 60 seconds. Hence, this difference leads to a drop of about 17 hours in the time duration required for solving the problem on a Pentium 4 (3 GHz) computer.

Another considerable point is that the optimized controllers are able to take the system under control in about 10 minutes with a maximum deviation of less than 1.5 °C from the set point, while the parameters used in the real plant control it with the deviation of around 1.4°C in 16 minutes.

7.1.2 Change in feed flow rate

In this case, the feed flow rate was reduced by 10%. The parameters derived for this change using the GA-SQP method are presented in Tab. 9. Temperature deviations can be observed in Fig. 4. At first, this change would result in a dramatic temperature rise at the outlet of exchangers. As a consequence of this growth, the inlet and so the outlet temperature of each reactor would increase.

Tab. 9 Parameters derived from GA-SQP for the second disturbance

Controller	K_P	unit	K_i	unit
PIC	1.961	1/bar	2.335	s^{-1}
TIC-1	1.741	1/°C	33.427	s^{-1}
TIC-2	0.357	1/°C	4.789	s^{-1}
TIC-3	0.363	1/°C	1.993	s^{-1}
TIC-4	0.367	1/°C	1.933	s^{-1}

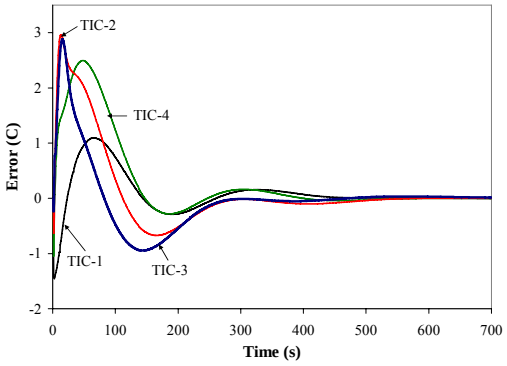

Fig. 4 Temperature deviation vs. time for second disturbance

It must be mentioned that the optimized set of controller parameters enables the controlling system to control the unit in about 5 minutes with maximum temperature deviation of less than 3°C, while the parameters used in the real plant control it with the deviation of around 2.9°C in 10 minutes. This problem was also solved with SQP and GA techniques and the same trend of the previous case was observed in reaching the final solution for the three methods.

7.1.3 Change in CO mole fraction

In this case it was considered that the carbon monoxide content of the feed would be doubled. The parameters obtained in this phase are illustrated in Tab. 10. The variation of temperature with time is shown in Fig. 5. This change would cause the reaction rates to decrease, and, therefore, a temperature drop would happen, because carbon monoxide leads the reaction rates to become slow.

Tab. 10 Parameters derived from GA-SQP for the third disturbance

Controller	K_P	unit	K_i	unit
PIC	1.962	1/bar	2.287	s^{-1}
TIC-1	1.742	1/°C	27.789	s^{-1}
TIC-2	0.357	1/°C	4.766	s^{-1}
TIC-3	0.362	1/°C	1.972	s^{-1}
TIC-4	0.367	1/°C	1.683	s^{-1}

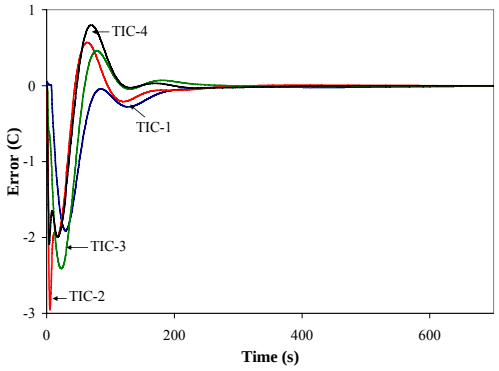

Fig. 5 Temperature deviation vs. time for third disturbance

In this case, using parameters used in plant results in controlling the disturbance in approximately 11 minutes with the deviation of around 2.8°C. On the contrary, as can be seen from the Fig. 5, with parameters obtained from optimization technique the disturbance is controlled in about 5 minutes with the deviation of about 3°C.

7.2 Choosing final control tuning parameters

As can be observed in Tabs. 6, 8 and 9, the parameters obtained from the algorithm are different from each other, though there is an ignorable difference between the parameters derived for cases 2 and 3. To determine the final set of the control tuning parameters, the second disturbance, i.e., decreasing the inlet flow rate, was used to test the first set of parameters derived from the first disturbance, which was decreasing the inlet temperature. The result is presented in Fig. 6. It is obvious that this set is not able to control this disturbance. On the other hand, the first disturbance, i.e., decreasing the inlet temperature, was used to test the second set of parameters derived from the second disturbance, which was decreasing the inlet flow rate. The result is revealed in Fig. 7. This set of parameters succeeded to control the disturbance with less temperature deviation, i.e., nearly 1°C, although in a longer time, which was 1000 s. This is in fact expected since the second set of parameters makes the controllers to become slower, which in turn, will result in less overshoot. Therefore, one can choose the second set as the final set of the controlling parameters.

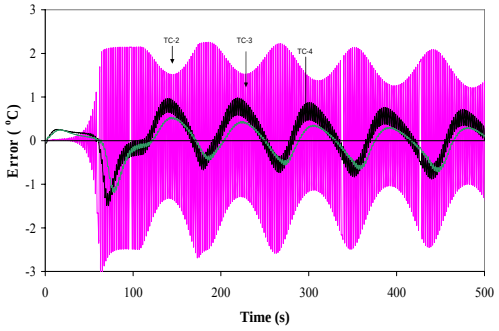

Fig. 6 Temperature deviation vs. time for the case of decreasing the inlet flow

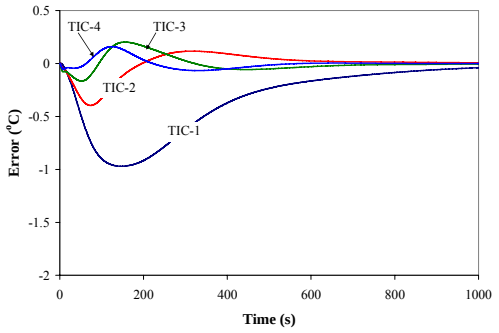

Fig. 7 Temperature deviations vs. time for the case of increasing the inlet temperature

8 Conclusions

Control tuning parameters of 5 PI controllers were determined the temperature and concentration data from an industrial hydrogenation unit. Stochastic methods, like the GA, are proper choices for solving such problems. However, deterministic methods, such as SQP, are not the proper choice for solving these kinds of problems. In fact, SQP is more vulnerable to get trapped in the local minima than the GA which has the ability of escaping from these points. However, the GA is generally slower than SQP. Therefore, the more robust GA with faster SQP were combined together in order to develop a robust and fast optimization technique. It was shown that the new GA-SQP hybrid method is able to determine the final solution considerably faster than the pure GA while it is not sensitive to the initial point.

9 Nomenclature

a	activity of catalyst
C	concentration (mol/m^3)
d	SQP independent variable
d_k	search direction
E	activation energy (J/mol)
E_a	apparent activation energy for catalyst deactivation
e	error
f	objective function (mol^2/m^6)
G	constraint function
H	Hessian matrix
K_i	Integral parameter in the function of controller (s^{-1})
K_p	Proportional parameter in the function of controller (%/error)
k_a	pre-exponent of catalyst deactivation rate constant (m$^{3\theta}$/ mol$^\theta$.s)
k_{Co}	adsorption constant for carbon monoxide
k_d	deactivation rate constant (s^{-1})
k_H	adsorption constant for hydrogen
k_i	reaction rate constant (m^6/mol.kg cat.s)
$k_{0,i}$	pre-exponential factor for reaction rate
L	Lagrangian function
m	number of constraints
m_e	number of equality constraints
R	gas constant (J/mol.K)
r_i	reaction rate for component i (mol/kg cat.s)
$r_{i,d}$	reaction rate for component i on deactivated catalyst (mol/kg cat.s)
T	temperature (K)
t	time (s)

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x vector of the control parameters

Greek letter

α step length parameter
ε bed voidage
θ order of apparent deactivation rate
λ multiplier vector
ρ_s catalyst density (kg/m^3)
υ penalty parameter
ψ merit function

Subscripts

CO carbon monoxide
Cte constant
f final time
H hydrogen
i component *i*
ind industrially measured value
j data point
k parameters related to quadratic space
l number of data point
m model predicted value
n number of components
s catalyst

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