

## Application of Genetic Algorithm to Identify Optimal Temperature Trajectory of a S-PVC Batch Reactor

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**Abstract:** This article discusses on development of a dynamic model for predicting transient behavior of a batch polymerization PVC reactor. It was utilized for increasing productivity of the polymerization process by minimization of its batch processing time. Genetic Algorithm (GA) was implemented for determining of the process optimal temperature trajectory profile to achieve a desired monomer conversion within a minimum batch time considering constraints of molecular weight and reactor thermal capacity. SQP method was initially implemented to improve the application of GA by generation of the first population of input data.

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**Keywords:** Poly Vinyl Chloride (PVC), Suspension Polymerization, Dynamic Optimization, Genetic Algorithm, Temperature Trajectory.

### 1. Introduction

Batch reactors have been widely used for production of materials including valuable and fine chemicals due to their flexible and economical operations. In polymer industries for having secure operations of batch reactors, more controllability and stability of them are required. Batch polymerization processes from both technical and academic point of view, are quite challenging. These are essentially due to the processes nature that usually involves: (i) a set of complex temperature-dependent chain reactions, (ii) high nonlinear behavior due to dependency reactions to concentrations and temperature, (iii) complex reactions' kinetic, and (iv) unsteady state conditions. In order to find the best operational conditions for having the highest performance, instead of applying a large number of trial & error operations that are tedious, time consuming, and consequently a costly operation, modeling of such processes and simulation of their behaviors under various operational conditions are an efficient approach. In such systems only a few state variable such as temperature and pressure are available for direct on-line monitoring and measurement. In order to increase the profitability of a batch polymerization system, besides of processing time, operating conditions such as temperature and pressure, should be optimized. This is an efficient approach to gain a maximum yield by minimizing of time and cost. This optimization enforces to have a specific processing condition for enhancing quality and quantity of products [1]. The quality of polymeric products can be evaluated by their average molecular weight and polydispersity

Index. These two important parameters of industrial batch polymerization reactor can be controlled based on design of advanced techniques in optimal control strategy.

Process optimization has significant impact on operability and economics of a polymerization plant. A set of research studies on optimization of polymerization systems was reported in literature which a list of them was provided by Silvia and Biscaia [2]. Most of these studies consider three following aims: (i) minimization of the reaction time as an objective function, (ii) reduction of monomers and initiators residues in products, (iii) maximization of monomer conversion and decreasing the deviation of the average number of chain length from its desired value [3, 4]. Based on computer-aided optimization, optimal operation strategies have employed for computation of optimal temperature profiles. Various researches were performed to show the effect of temperature on polymerization in order to gain maximum yield or desired final product specifications [5]. Manipulating operational variables are usually temperature, concentrations of initiator additive and monomer.

Classical analytic methods for optimization such as direct search and gradient-based approach have been usually implemented to solve problems in process engineering. The main weaknesses of these methods are [2, 6]:

- Incapability of finding the global optimal in a non-monotonic search space,
- high dependency of converged solution as the optimal value to selected initial solution,

- tends for sticking to a sub-optimal solution in most of algorithms,
- lack of an efficient algorithm for solving various optimization problems, and
- prerequisite to a large number of systems' information, such as initial guess and derivatives of objective function to guide a search strategy.

In recent years, due to the rapid progress for fast computation in both hardware and software technologies, advanced numerical search algorithms have become more popular. In particular, there have been growing interests on genetic and evolutionary algorithms for optimization problems. These methods are robust, flexible, reasonably fast, capable to find solutions quite close to global optima, and without any need to a suitable initial guesses for converging to a global optimum solution.

Genetic algorithm (GA) is a mathematical optimization technique that simulates a nature evolution process. GA is a powerful search technique based on the mechanics of natural genetics and natural selection. Since development of GA by John Holland in 1975, it has been constantly implemented for solving of various optimization problems and industrial applications [6]. This technique were applied to field of process engineering to predict an optimal temperature trajectory for minimizing reaction time of producing resins with a desired molecular and morphological properties in a safe, easy and efficient way [3].

In our study, initially a comprehensive mathematical model was designed and developed. It was based on transient mass and energy balances implementing supplied data of Kiparissides et al. [7]. After validation of the created model, it was utilized to simulate the reactor behavior, and in conjunction with GA, it was implemented for identification of optimal temperature history profile. This profile minimizes of the polymerization batch time, and employs maximum cooling capacity of the reactor. Meanwhile it provides desired final product conservation, and the average molecular weight of product.

## 2. Process description and modeling

This section explains the PVC polymerization system, the model basic information, and model validation.

### 2.1 Process description

PVC is one of the oldest polymers and the second largest manufactured thermoplastic in the world that its demand is growing. There are varieties of processes for production of this polymer. Suspension process is the most important method for manufacturing of a range of either general purpose, or highly sophisticated grade of PVC. Vinyl Chloride

Monomer (VCM) is normally polymerized in a batch reactor by dispersing of the liquid monomer in water under pressure and intense agitation [7]. The polymerization reaction takes place in the suspension droplets and is initiated in presence of one or more initiators. Initiators are normally added in a single stage only. Peroxides have typically been used for initiation. The reactor's contents are heated to a certain temperature for decomposing of the initiator(s) and commencing polymerization. Decomposition of initiators for suspension PVC polymerization has usually a relatively slow kinetics. The reaction of PVC polymerization is highly exothermic, and the production rate is limited by available cooling capacity. The heat of polymerization is transferred from the monomer droplets to the bulk water phase and then to the reactor wall, which is cooled by water flowing in the reactor's jacket [1]. Hence, the design of an efficient cooling system is a major concern. Since PVC is mostly insoluble in its monomer, once the polymer chains are produced, they precipitate immediately and form a separate phase within polymerization droplets. Reactions are carried out in the both free liquid monomer-rich phase and entrapped monomer in the polymer-rich (gel) phase, which is dispersed about the formed polymer. By consumption of free liquid monomer, the reactor pressure drops due to transfer of monomer from the vapor phase to the polymer-rich phase as a result of sub-saturation conditions. By completion of polymerization process, the produced polymer is in the form of dispersed particles in water.

### 2.2 Model description

Reaction kinetics, kinetics parameters, thermodynamics data, and physical properties of the PVC suspension batch reaction were taken from Kiparissides et al. [7]. Table 1 represents the kinetics

scheme for PVC polymerization. Symbols  $I$ ,  $M$ ,  $R_x$ ,  $P_x$ , and  $Z_j$  denote initiator, monomer molecules, live macro radicals and dead polymer chains containing  $x$  monomer units, and inhibitor radicals, respectively. Parameter of  $N_d$  represents the number of initiators in the polymerization process, and the subscript  $j$  refers to the phases, i.e.  $j=1$  for the monomer, and  $j=2$  for the produced polymer.

All of the bellow reactions, except the one for the chain transfer to polymer, are modeled as they occur in both monomer and the gel phase. The reaction of chain transfer to polymer occurs only in the gel phase. Reaction kinetics, diffusion, controlled termination, and propagations have been related to the well-known phenomena of gel and glass effects in the suspension polymerization of PVC. The gel effect

arises due to decreasing of termination rate constant at high monomer conversion, associated with increased diffusion resistance as a result of growing radicals. The glass effect is associated with reduction in propagation rate constant that is due to increasing of

diffusion resistance in transferring of monomer toward growing radicals. This leads to stop the polymerization and complete monomer conversion, even though the reactions to be irreversible.

Table 1. Kinetic mechanism for polymerization of PVC [7].

Decomposition of initiator	$I_{ij} \xrightarrow{k_{iz}} 2I_{ij} \quad i=1, 2, \dots, N_d$
Generation of polymer radicals	$I_{ij} + M_j \xrightarrow{k_{ij}} R_{ij}$
Propagation	$R_{x,j} + M_j \xrightarrow{k_{pj}} R_{x+1,j}$
Chain transfer to monomer	$R_{x,j} + M_j \xrightarrow{k_{fmj}} P_x + R_{1,j}$
Chain transfer to polymer	$R_{x,2} + P_y \xrightarrow{k_{fp2}} P_x + R_{y,2}$
Termination by disproportionation	$R_{x,j} + R_{y,j} \xrightarrow{k_{idj}} P_x + P_y$
Termination by combination	$R_{x,j} + R_{y,j} \xrightarrow{k_{icj}} P_{x+y}$
Back-biting reaction	$R_{x,j} \xrightarrow{k_{bj}} R_{x,j}$ $Z_j + Z_j \xrightarrow{k_{zj}} Z_j + \text{Inactive Products}$

Dynamic mass balance equations for the calculation of the time variation of initiator and total monomer conversion can be expressed in following form [7]:

$$\frac{d[I]_{i,1}}{dt} = -k_{d,i} [I]_{i,1} ; \quad i = 1, 2, \dots, N \quad (2.1)$$

$$[I]_{i,2} = K_{I_i} [I]_{i,1} \quad (2.2)$$

$$\frac{d[Z]_j}{dt} = -\frac{1}{2} \sum_{j=1}^2 k_{Z_j} [Z]_j [\lambda_{0,j}] \quad (2.3)$$

$$\frac{d[X]}{dt} = \sum_{j=1}^2 k_{p_j} \frac{M_j}{M_0} [\lambda_{0,j}] \quad (2.4)$$

where I, Z, and X are initiator concentration, inhibitor concentration, and conversion factor, respectively. Parameter  $K_{I_i}$  is initiator distribution coefficient and its value is estimated experimentally.

Coefficients of  $k_{d,i}$ ,  $k_{z_j}$ , and  $k_{p_j}$  are decomposition rate constant for i-th initiator of in j-th phase, inhibition rate constant in j-th phase, and propagation rate constant in j-th phase, respectively. Parameter  $\lambda_{i,j}$  is i-th moment of molecular weight distribution of live polymer radicals in phase of j.

Polydispersity index (PDI) which is a measure of the breadth of molecular weight distribution. It is defined as the ratio of average weight to number average molecular weight. It indicates the distribution

of individual molecular masses in a batch of polymers. Values of PDI are affected by the mechanism of polymerization, and the conditions of reaction.

Details of developed model including dynamic energy balance and relevant data are not described in detail as the scope of this article is presentation of results on application of GA for finding optimal temperature history profile.

### 2.3 Model validation

The developed model was used to simulate a batch polymerization reactor with 1.5 liters initial charge of VCM, 1.5 liters of water, and 1.57 grams of dilauroyl peroxide per kg of VCM at isotherm of 63°C. The model's differential equations were solved by fourth-order Runge-Kutta method. Dynamic

simulation results of the reactor consisting of monomer conversion, reactor pressure and polymerization rate are shown in figure 1. Also corresponding data from Kiparissides et al. [7] are represented to provide a better comparison for validating of the developed model.

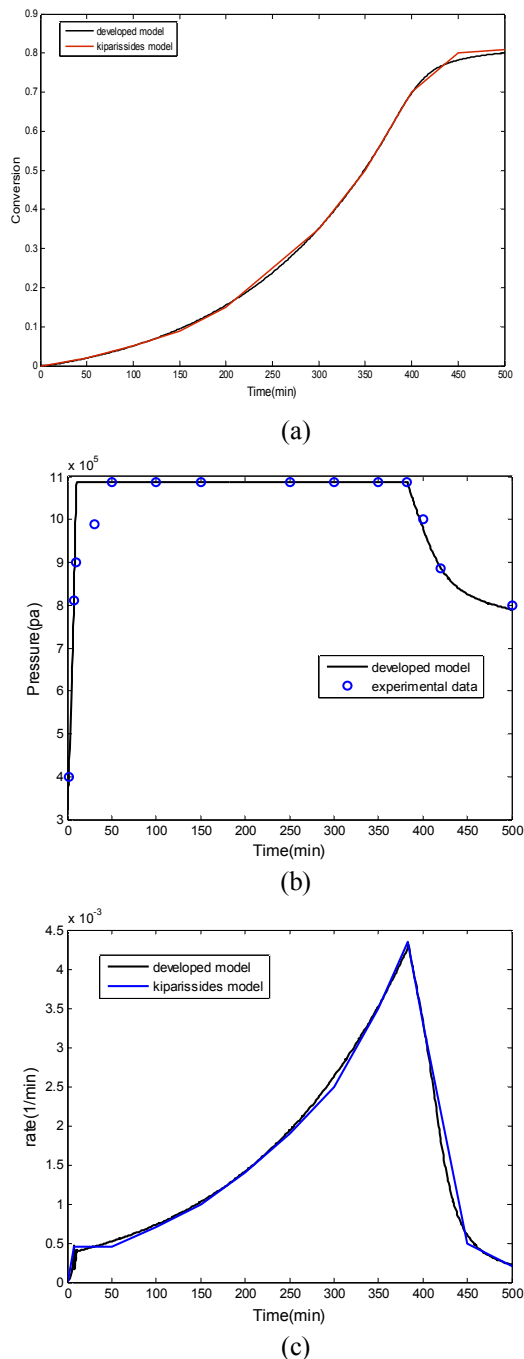


Fig. 1. Comparison of the simulation results with published data of Kiparissides et al. [7], (a) monomer conversion, (b) reactor pressure, and (c) reaction rate, (in presence of the one initiator).

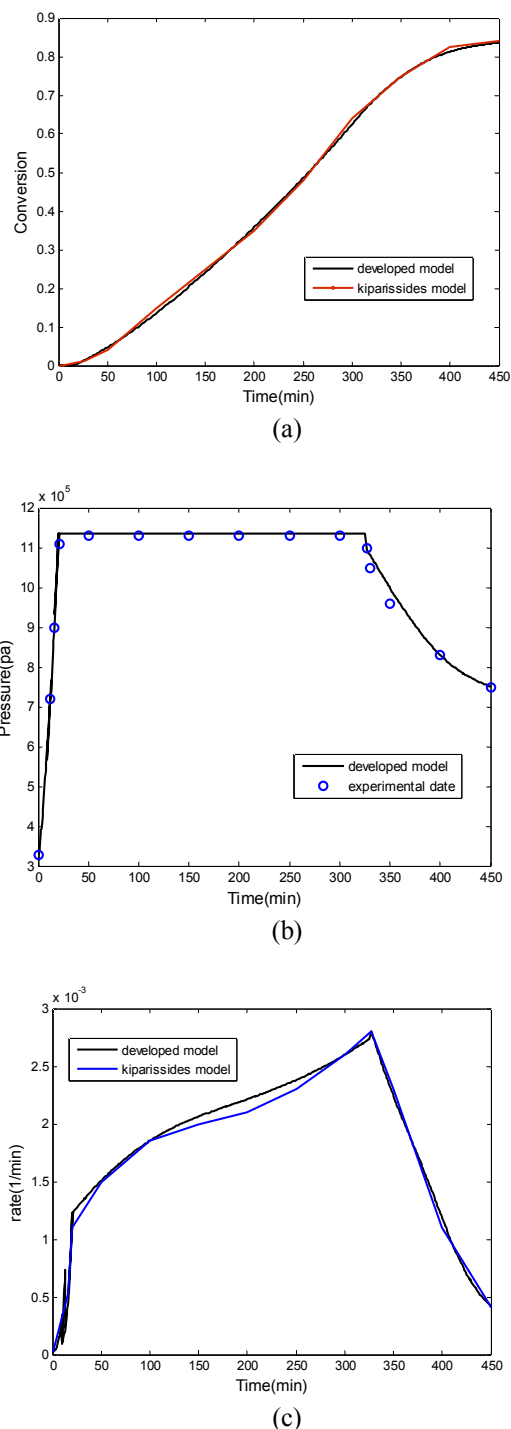


Fig. 2. Comparison of the simulation results with published data of Kiparissides et al. [7], (a) monomer conversion, (b) reactor pressure and (c) reaction rate, (in presence of the two initiators).

It should be noticed that in figure 1(b) the simulated pressure of reactor is compared with the experimental one. While in other two plots of this figure, simulation results of the two models are

compared. The slight mismatches of the results in these two plots are due to differences in some data used in the developed model and Kiparissides et al. model [7]. These data those are essential for developing of the model. They were acquired based on laboratory works and was used in the Kiparissides et al. model. They were reported neither in the published paper nor in other resources. Thus, these data such as solubility data of initiator in phases, parameters in diffusion-controlled phenomena, such as radius of a monomer molecule, and the monomer diffusion coefficient were obtained through curve fitting, and trail and error methods.

Furthermore, the developed model was verified by simulation of a polymerization reactor with following ingredients: 2.12 liters initial charge of VCM; 2.34 liters of water; and a mixture of 0.35 g of dilauroyl peroxide, and 0.17 g of diethyl peroxidicarbonate per kg of VCM; at isotherm of 64°C.

Transient conversion of monomer, reactor pressure, and polymerization rate are shown in figure 2. These results were compared with corresponding data of Kiparissides et al. [7].

As mentioned the origin of slight difference in simulation results of the two models are due to discrepancy of assigned data for unknown parameters of the developed model.

### 3. Genetic Algorithms

Genetic Algorithm is a stochastic global search method that has been used widely. It is a mathematical optimization technique based on the Darwinian Theory, in which the fittest species survive and propagate while the less successful tend to disappear [8]. GA starts with no knowledge of the correct solution and performs parallel searching at several independent points. Genetic algorithm avoids local minima and converging to the best solution based on environment and evolution operators. This algorithm evolutionary strategy consists of performing genetic operators on a random population to generate the next population. The search is progressed generation by generation, guided by an individual fitness evaluation, which is based on a ranking procedure [8]. It is capable of working in complex multi-dimensional domains without difficulty [9].

Steps in implementing of a genetic algorithm for finding optimum are in following sequences:

1. Generating a random and fixed size population of individuals, initialization.
2. Evaluate of their fitness.
3. Select the fittest members of the population.
4. Reproduction, using a probabilities tic method (e.g., roulette wheel).

5. Implement crossover operation on the reproduced chromosomes (choosing probabilistically both the crossover site and the 'mates').
6. Execute mutation operation with low probability.
7. Repeat the second step until meeting of a predefined convergence criterion.

Figure 3 illustrates the flow diagram of these stepwise operations.

The convergence criterion of a genetic algorithm is a user-specified condition, e.g. the maximum number of generations or when the string fitness value exceeds a certain threshold.

In order to stop the sequence of successive population generations, a termination criterion based on the convergence of the evolutionary process is adopted. The termination criterion consists of the evaluation of the best solution of each individual objective function. It should be emphasized that the adopted parameters in the termination criterion are chosen after a careful monitoring of the algorithm evolution. Therefore, verification for sufficient number of generations for the convergence was necessary. The values of parameter depend on the complexity of the problem and the required accuracy. At each generation, the evaluation of the objective functions is performed once for each point. Thus, the performance of the algorithm should be inferred from the number of model simulations, instead of the number of objective function evaluations. The total number of model simulations is calculated as follows:

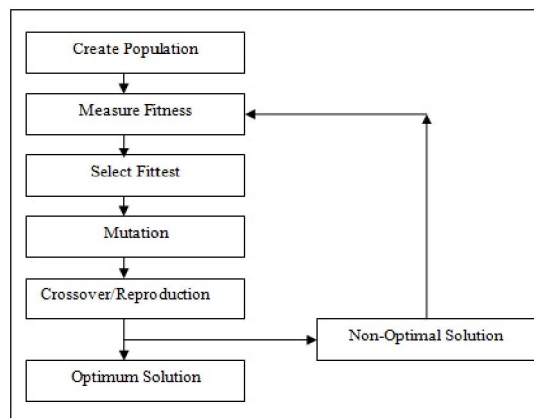


Fig. 3. Flowchart of the implemented genetic algorithm [2].

$$n_{\text{mod\_eval}} = n_{\text{gen}} \times P_s \quad (3.1)$$

where  $n_{\text{gen}}$  is the maximum number of generations, and  $P_s$  is population size [2].

The fitness evaluation at each point of the population is the only information that is required by GAs to conduct the search.

#### 4. Description of the GA model

In GA model of this research, a binary solution was used in order to encode the chromosomes. More natural encoding such as value encoding and tree encoding is more efficient and has better solutions. A population of 20 individuals was used in this work as increasing the population size does not improve the performance of implemented GA. A suitable population size has reported in the range of 20 to 100 individuals [8]. In reproduction stage, a roulette wheel selection was used for selecting parents that are proportional to their fitness. In this work, a two-point crossover with a probability of 0.8 was used. After generating of a new individual, a mutation operator with a probability of 0.05 was performed over it. The probability of mutation is normally low, as in a high mutation rate, generation of fitted strings would be destroyed and put the GA into a random search.

#### 5. Formulation of dynamic optimization

A mathematical model based on the mechanism of free radical polymerization was developed to describe the process behavior. Simulation of the polymerization system is required to evaluate the individuals in terms of the objective function and constraints. This is used for optimization of the batch polymerization system. At each step of optimization procedure, the stiff differential equations of the model were generated and solved.

The target was finding of a product to cover followings:

- A desired monomer conversion ( $X_d$ ),
- a desired value for the average molecular weight number ( $Mn_d$ ),
- the most usage of reactor thermal capacity for removal of the polymerization process heat, and
- determination of the non-isothermal temperature profile for having maximum conversion in a minimum reaction time.

Consider the optimization problem based on objective function of  $J$  as:

<b>Minimize (<math>J = t_f</math>)</b>
Subject to:
Process model: $\frac{dx}{dt} = f(x(t), P, T, t)$ .
Initial condition: $x(t_0) = x(0)$ .
Constraints: $\left\{ \begin{array}{l} 35^\circ\text{C} \leq T_r \leq 75^\circ\text{C} \\ Q \leq H_r \\ X(t_f) = 0.88 \\ Mn(t_f) < Mn_d \end{array} \right.$

#### 6. Results and discussion

The objective function in the first investigation and according to the specified constraints in GA, in various temperatures had the same results. It was remained constant in long time until to achieve minimized reaction time. In fact, GA must search a big flat space to find global optimal in a convex area. As a result, the objective function had zero derivation with respect of time. It was a derivable function and therefore other optimization method such as Sequential Quadratic Programming (SQP) that is used with derivable objective functions and has a proper convergence speed to find optimum trajectory temperature and reduce the computation time and cost of GA, was necessary. SQP reduces the required number of objective function evaluations for convergence to an optimum [6, 10].

SQP technique mimics Newton's method for constrained optimization in that at each major iteration an approximation is made of the Hessian of the Lagrangian function using a quasi-Newton method. This is used to generate a QP sub-problem whose solution is used from a search direction for a line search procedure. In this study, optimization algorithm by using SQP method is started until achieving a local point in searched area, then obtained results from SQP as an initial point for GA.

In the first case study, optimization was performed for the developed model based on one initiator. A set of 12 runs based on the present constraints in table 3 was designed. By achieving the reactor thermal capacity constraint, the initial temperature trajectory point was set to 75 °C. Higher temperature results in destroying of VCM.

Temperature trajectory of the run # 1 is shown in figure 4. Concentration of radicals in the first stage is low, as the reaction just takes place in monomer suspension droplets - rich phase. Thus, increasing of conversion factor with respect to time is low. Also, the process temperature stays in upper limit temperature (75 °C) for few minutes without affecting of the average molecular weight. By progressing of the reaction in second stage of polymerization, the separated polymer phase appearances and reaction takes places in both phases. Free radical polymerization reaction is exothermic and has the same behavior as autocatalytic reaction. Therefore, with progress of polymerization, the rate of reaction was increased and then the system temperature was reduced to use the maximum thermal capacity of reactor to transfer heat of reaction. Finally, monomer phase was completely used and reaction took place only in polymer-rich phase. This was led to increase the temperature in the third stage and improves VCM conversion.

Table 2. Constrains of designed optimization runs (1 initiator)

run #	Q (KJ/min)	Mn <sub>d</sub>
1	Less than 9	
2	Less than 8.1(-10%)	
3	Less than 7.1(-20%)	
4	Less than 9	Less than 32000
5	Less than 9	Less than 35200(+5%)
6	Less than 9	Less than 28800(-5%)
7	Less than 8.1(-10%)	Less than 32000
8	Less than 8.1(-10%)	Less than 35200(+5%)
9	Less than 8.1(-10%)	Less than 28800(-5%)
10	Less than 7.1(-20%)	Less than 32000
11	Less than 7.1(-20%)	Less than 35200(+5%)
12	Less than 7.1(-20%)	Less than 28800(-5%)

In run # 4 to run # 9, the profiles trends were same as shown in figure 4. In run # 10 to run # 12, GA could not search points of temperature that minimizes the objective function within the range of defined constraints.

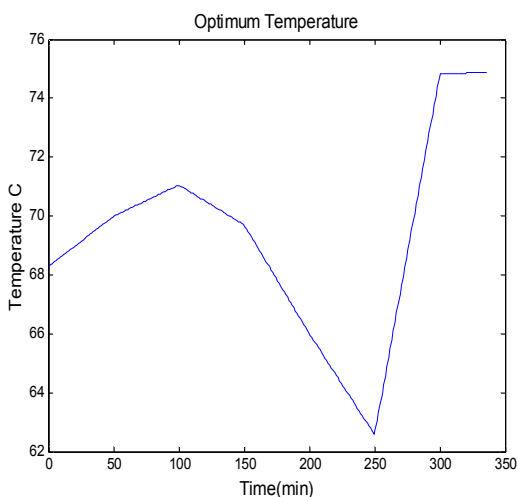


Fig. 4. Temperature trajectory of the run # 4 based on GA optimization (Initial reactor charge: 1.5 L VCM; volume water; 1.5 L and 1.57 g of dilauroyl peroxide/Kg of VCM).

Variation of generated reaction heat with respect to time base on the obtained temperature trajectory is shown in figure 4. In the second stage, reactor uses maximum reactor thermal capacity depending on temperature track. The total pressure of reactor was reduced based on optimization temperature profile as shown in figure 5. In run # 2 obtained profiles have the same trend as run # 1. In run # 3 GA could not minimize final time to satisfy the specified constraint.

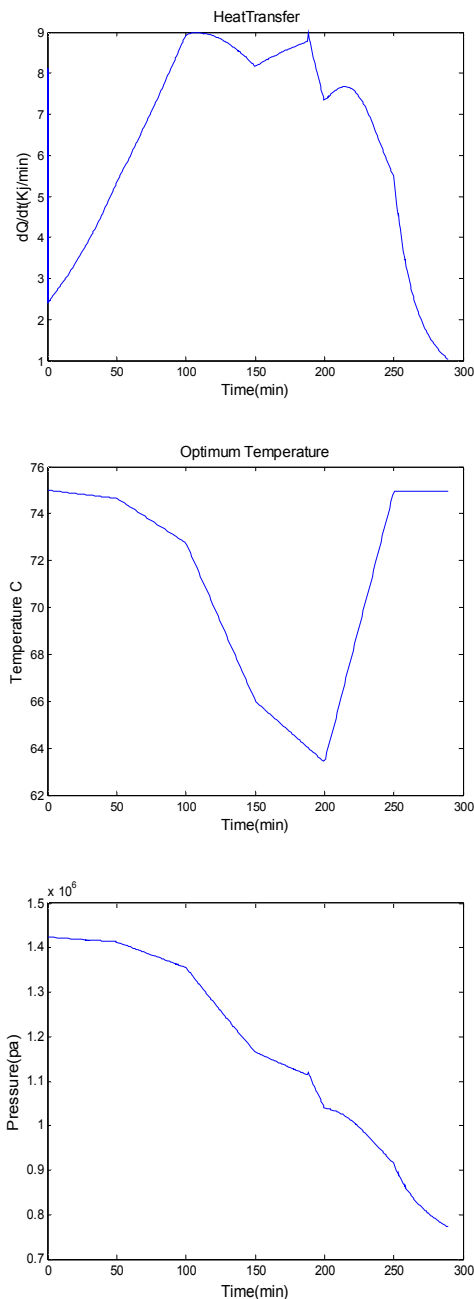


Fig. 5. Temperature trajectory, reactor thermal capacity, and total pressure reactor of the run # 1 based on GA optimization (Initial reactor charge: 1.5 L VCM; volume water; 1.5 L and 1.57 g of dilauroyl peroxide/kg of VCM).

By application of genetic algorithm for reducing of reaction time to reach conversion of 88% for all of specified runs from run # 1 to run # 9 in tables 3 is presented. It shows that genetic algorithm is managed to reduce reaction time by using specified constraints as well as reaching high conversion.

Table 3. Optimization results of reaction condition for reaching to conversion of 0.88 for monomers.

run #	Minimized time of reaction (min)	Mn	PDI (Non-isothermal optimization)	PDI (Isothermal optimization)
1	289	28446	2.206	2.452
2	337	29494	2.233	2.393
4	336	28867	2.222	2.431
5	346	28640	2.228	2.440
6	349	28232	2.295	2.464
7	401	28951	2.313	2.425
8	341	29105	2.257	2.448
9	450	28699	2.377	2.608

In table 4, the percent of improvement reaction time for non-isothermal condition in order to reach  $X=0.8$  in comparison with developed model of final time reaction (500 min) is shown. Also investigations and comparisons about polymerization reaction show that time for model Kiparissides et al. at isothermal temperature ( $T=63\text{ }^{\circ}\text{C}$ ) to reach conversion of 0.8 takes a long 500 minutes but reaction time for reaching this conversion has been decreased considerably in non-isothermal optimal temperature track.

Table 4. Optimization time for reaching to conversion of 80% for monomer

run #	reaction time (min)	Improvement time (%)
1	238	52
2	288	42
4	286	43
5	286	43
6	288	42
7	343	31
8	288	42
9	385	23

Number average molecular weights of polymers (Mn) based on optimization operations and specified concentrates of run # 1 to run # 9 under isothermal and non-isothermal conditions are presented in table 3. As the desired value of the number average molecular weight increase, the reaction takes longer time. It can be seen the polydispersity index under isothermal condition is higher than non-isothermal condition. High polydispersity index leads to widen distribution of the average molecular weight of produced polymer. Polydispersity index was decreased by reducing of polymerization time. As the global of the polymerization process is to produce a polymer with desired physical properties, polydispersity index about 2 at a minimum process time, it is recommended to have reaction under non-isothermal condition based on an optimized historical trend. The temperature trajectory under various concentrates for number average molecular weight was shown the best PDI characteristic for produced

polymer based on optimization under condition non-isothermal in comparison to isothermal condition, In order to have the same the number average molecular weight.

With comparisons of results under various conditions and results in tables 3 and 4, it can be concluded that GA should search in a more limited domains by reducing of domain of constraints for thermal capacity of reactor, and number average molecular weight. Therefore, GA is not able to reduce reaction time in some domains of temperature, see results of run # 9.

In the second case study, the optimization process was performed for two initiators using in developed model. A set of 12 runs was designed with specified constraint as shown in table 5. In this case, initial start point for trajectory temperature for all runs varies between 35 to 75  $^{\circ}\text{C}$ .

Table 5. Constrains of designed optimization runs (2 initiators)

run #	Q (KJ/min)	Mnd
13	Less than 7.5(-10%)	-
14	Less than 8.3	-
15	Less than 6.7(-20%)	-
16	Less than 8.3	Less than 34600
17	Less than 8.3	Less than 3806(+5%)
18	Less than 8.3	Less than 31140(-5%)
19	Less than 7.5(-10%)	Less than 34600
20	Less than 7.5 (-10%)	Less than 38060(+5%)
21	Less than 7.5(-10%)	Less than 31140(-5%)
22	Less than 6.7(-20%)	Less than 34600
23	Less than 6.7(-20%)	Less than 3114(+5%)
24	Less than 6.7(-20%)	Less than 38060(-5%)

The obtained optimum temperature trajectory in run # 13, leads to reduce batch polymerization time in non-isothermal condition while maximizing the usage of available reactor cooling capacity is presented in figure 6. In other runs, obtained profiles have same trend as run # 13. The same trend in profiles of run # 13 to run # 24 has obtained that has shown in figure 6. In run # 15, run # 17, run # 18, and run # 21, GA



could not minimize the objective function in range of defined constraints.

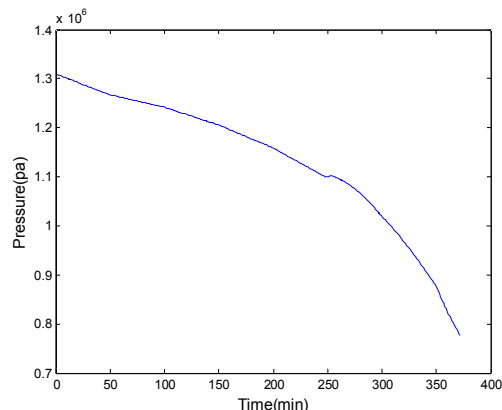
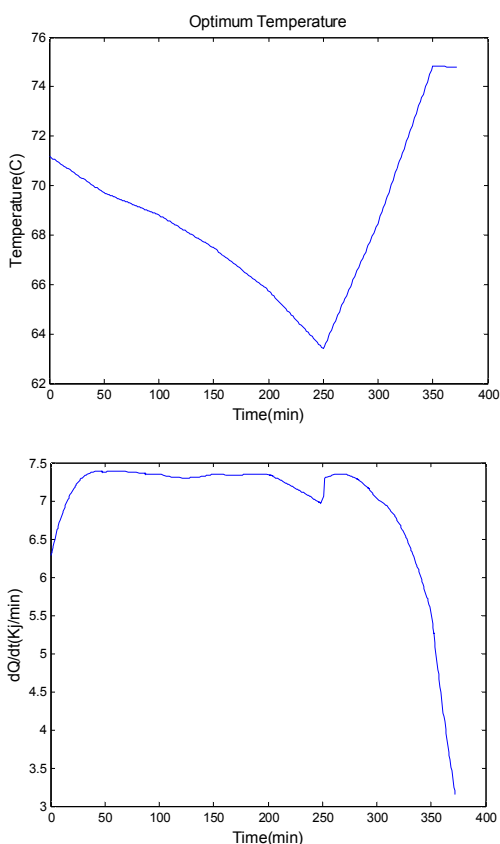


Fig. 6. Temperature trajectory, reactor thermal capacity and total pressure reactor of the run # 13 based on GA optimization (Initial reactor charge: 2.12 L VCM; 2.34 L water; 0.35 g of dilauroyl peroxide/Kg of VCM and 0.17 g of diethyl proxydicarbonate/Kg of VCM).

The optimization result based on GA is presented in table 6. It shows, that by setting of the desired monomer conversion to  $X_d = 0.88$ , the temperature trajectory for various limit of number average molecular weight, reaches to a better value for PDI in comparison with one initiator. By reduction of the minimum reaction time, the PDI property was decreased which state a narrow molecular weight distribution for the product.

Table 6. Optimization results of reaction condition for reaching to conversion of 0.88 for monomers

run #	Minimized time of reaction(min)	Mn	PDI(Non-isothermal optimization)	PDI(Isothermal optimization)
13	372	34485	2.032	2.123
14	427	39500	2.035	2.064
16	445	34600	2.090	2.121
19	427	37200	2.081	2.121
20	412	34590	2.045	2.098
22	402	28951	2.047	2.121
23	423	31133	2.140	2.168
24	448	37956	2.063	2.086

Table 7. Progress decrease time by GA in comparison reference model,  $X=0.84$ ,  $t=450$  min

run #	Reaction time (min)	Improvement (%)
13	347	23
14	420	7
16	387	14
19	374	16
20	389	42
22	364	19
23	321	29
24	419	7

The percent of improvement reaction time in non-isothermal condition in order to reach  $X=0.84$  in comparison with developed model of final reaction time is presented in table 7.

## 7. Conclusion

A mathematical model for batch polymerization reactor of PVC was developed based on mass and energy balance. The model was used to simulate the behavior of the reactor that was in good agreement with the published experimental data. GA was used to find global optimal temperature histories of PVC

polymerization that uses maximum available reactor cooling capacity and minimum reaction time.

Application of GA and developed model leads to specify an optimal temperature trajectory to produce a polymer with a desired specification on molecular weight and reaction conversion. Operating the S-PVC batch reactor in track of non-isotherm optimal temperature trajectory led to reduction of the polymerization process batch time while maximizing the usage of available reactor cooling capacity. Produced polymer has desired molecular and morphological properties with a narrow molecular size distribution. Furthermore, by following the optimal temperature trajectory, the economic yield increased by reduction of operating time. This technique could easily be used for on-line optimizing control of experimental reactors.

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