

A Novel Real-time Optimization Methodology for Chemical Plants

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Abstract In this paper, a novel approach termed process goose queue (PGQ) is suggested to deal with real-time optimization (RTO) of chemical plants. Taking advantage of the ad-hoc structure of PGQ which imitates biologic nature of flying wild geese, a chemical plant optimization problem can be re-formulated as a combination of a multi-layer PGQ and a PGQ-Objective according to the relationship among process variables involved in the objective and constraints. Subsequently, chemical plant RTO solutions are converted into coordination issues among PGQs which could be dealt with in a novel way. Accordingly, theoretical definitions, adjustment rule and implementing procedures associated with the approach are explicitly introduced together with corresponding enabling algorithms. Finally, an exemplary chemical plant is employed to demonstrate the feasibility and validity of the contribution.

Keywords real-time optimization, chemical plants, process goose queue, multi-layer process goose queue

1 INTRODUCTION

A chemical plant is consisting of a series of interconnected operational units in which downstream units are influenced by upstream units, or mutually. From a mathematical programming perspective, process optimization refers to a nonlinear programming problem subject to process variable constraints stemmed from process models. By real-time optimization (RTO), it means that after online recognizing and analyzing the influences of uncertain disturbance on the economic objective functions, timely intervention is made to adjust operational conditions, keeping processes going on ideally in terms of economy performance. Traditionally, RTO approaches can be classified into two relatively distinct categories in terms of process model architectures: global or centralized architecture and decentralized architecture. The existing enabling algorithms for global architecture include penalty function methods, feasible direction methods, sequential quadratic programming and so on, which have been widely circulated in various research fields [1–3]. Alternatively, evolution algorithms such as genetic algorithm, particle swarm optimization and ant colony algorithm could be put in use concerning increasing complexity of optimization problems [4–6]. However, those global optimization algorithms were flung into dilemmas in the face of chemical plants. The main impacts on global optimization performance in chemical plants may arise from model complexity and nonlinearity, as well as heavy computational burden due to enormous manipulated variables involved. Instead, decentralized approaches decompose complex optimization problems into several sub-systems mutually coordinated. Relevant to this research, Dantzig-Wolfe decomposition [7] has been proved quite active in solving process optimizations [8, 9]. However, limited to deal with linear programming problems, Dantzig-Wolfe decomposition is less adapted for processes which usually involve severe nonlinearity. In a parallel study, Lagrange

multiplier approaches have attracted much attention as well, which firstly convert an optimization problem into a multi-system and subsequently deal with it using coordination parameters. The approaches include interaction prediction methods, interaction balance methods and interaction prediction and balance methods [10, 11], which offer theoretical supports for decomposition and coordination optimization of chemical plants [12]. Nevertheless, the added Lagrange multipliers increase the calculation burden, furthermore, demanding for separable or approximately separable objectives, the above-cited methods are more susceptible to considerable systematic deviations in the presence of severe nonlinear relations between the global objective and sub-objectives.

Actually, a chemical plant can be recognized as the connections of numerous basic operational units, which are considered as dynamic systems constituted by output process variables and input process variables. Inspired by nature of flying goose queue, a certain kinds of operational units could be regarded as a goose queue so that the achievements of optimum set-points of operational units are consistent with the mechanism of a flock of geese self-organizing into the optimum V-formation. In line with this thought, a novel idea of “process goose queue (PGQ)” is proposed to reconfigure chemical plants, thereby optimizing them in terms of economic perspectives. With the PGQ methodology, chemical plant models can be decomposed hierarchically according to goose queue formation, resulting in a multi-layer process goose queue. RTO for a chemical plant is therefore converted into PGQ follow-up and PGQ-Objective achievement steps governed by adjustment rules associated with a PGQ.

2 PROCESS GOOSE QUEUE METHODOLOGIES

The underlying philosophy of a flying goose queue has been studied by several researchers [13, 14],

Received 2012-05-16, accepted 2012-07-10.

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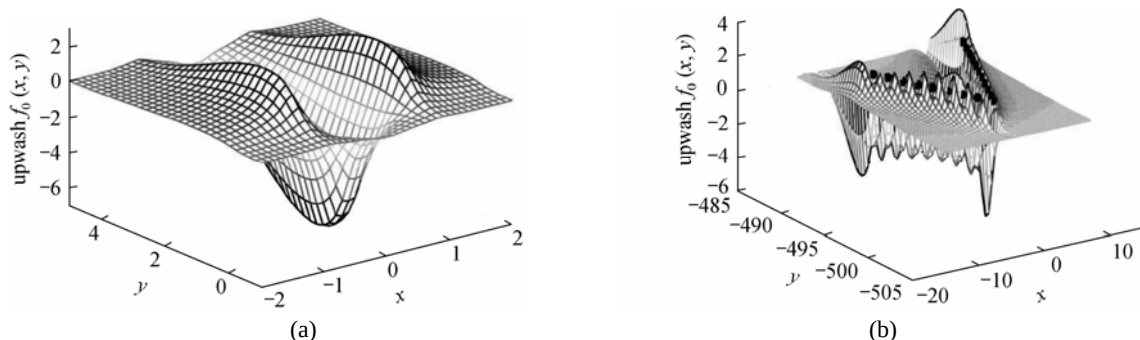


Figure 1 Illustration of (a) upwash generated by a flying goose and (b) formation of a goose queue

leading to corresponding upwash models. A flying goose could generate a position related upward pressure known as upwash, which is beneficial for following geese both in maintaining altitudes and saving energy. Assuming that the wingspans of all birds are constant and the upwash function (f_0) which is the function of position (x, y) is convex, an optimum position is available where the upwash is maxima as shown in Fig. 1 (a). Every following goose should take the optimum position as objective and achieve the optimal position by measuring the upwash and communicating with their neighbors. The eventual steady-state formation is shown in Fig. 1 (b).

From operation perspectives, a chemical plant can be recognized as connections of a variety of basic operational units. Generally, steady-state relationship among the basic operational units of the chemical plant can be described by following equation:

$$\mathbf{Y} = g(\mathbf{S}, \mathbf{X}) \quad (1)$$

where, $\mathbf{Y}$, $\mathbf{S}$, $\mathbf{X}$ and g indicate sets of the output state variables, input state variables, manipulated variables and steady-state relationship functions, respectively. In this sense, we could offer basic descriptions associated with PGQ approaches.

Definition 1 PGQ

A process goose queue (PGQ) is a 3-tuple, $\text{PGQ} = (L, F_S, F_M)$, where L is the leading goose position (LGP), such that $[(L | L \subset \mathbf{S}) = \emptyset]$, represented as (L) ; F_S is the state following goose position (SFGP), such that $F_S \subset \mathbf{S}$ represented as (F_S) ; F_M is the manipulated following goose position (MFGP), such that $[(F_M | F_M \subset \mathbf{X}) \neq \emptyset]$, represented as (F_M) ; and $F_S \cap F_M = \emptyset$, $L \cap F_M = \emptyset$, $L \cap F_S = \emptyset$.

The graphical description of a PGQ is illustrated in Fig. 2, where the leading goose position (L), state

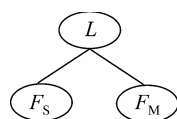


Figure 2 A PGQ (process goose queue)

following goose position (F_S) and manipulated following goose position (F_M) represent output process variables, $\mathbf{Y}$, input process state variables, $\mathbf{S}$, and input process manipulated variable, $\mathbf{X}$, respectively.

Definition 2 Optimum formation

An optimum formation, $\text{PGQ}^* = (L^*, F_S^*, F_M^*)$ refers to an ideal PGQ formulation in which every goose of the PGQ can benefit from the maximum upwash, where $*$ denotes the optimum value.

Practically, optimum operating states could be destroyed by uncertain disturbances, which perturb LGP from the ideal trajectory or cause the SFGP and a MFGP to be different from upwash maxima. All those situations will lead to inferior operating states and are in desperate need of adjustment to recover. Motivated by this idea, two alternative adjustment rules associated with a PGQ are specified as follows.

Rule 1 SFGP driven adjustment

Once the operating state of PGQ deviates from an optimum one due to SFGP failing to follow it, MFGP would try to adjust its position autonomously to formulate a new optimum formation. At the same time, LGP would slightly shift its position to survive the adjustment of MFGP. This kind of adjustment implies solving the following optimization problems.

$$\begin{aligned} & \min_{F_M} (L^* - L)^2 \quad (2) \\ \text{s.t. } & L = f(F_S, F_M) \\ & L_L \leq L \leq L_U \\ & F_{ML} \leq F_M \leq F_{MU} \end{aligned}$$

where f corresponds to the relationship among LGP, SFGP and MFGP.

In regard to Rule 1, the case of SFGP failing to follow optimum operating state is equivalent to the emergence of the uncertain disturbances in process, and L will be driven back to ideal trajectory by manipulating F_M , keeping F_S constant and utilizing steady-state relationship function $L = f(F_S, F_M)$. Therefore, Rule 1 can be adopted as adjustment rule in chemical plant RTO mentioned in this paper.

3 REAL-TIME OPTIMIZATION

3.1 PGQ formulations

In fact, process optimization could be identified as a procedure of adjusting manipulated variables to minimize or maximize economic goals subjecting to the constraints of process models.

The fact that chemical plant models depend on the connections of operational units accounts for hierarchical decompositions of process models, which is described as a multi-layer PGQ.

Definition 3 Multi-layer PGQ

A multi-layer PGQ consists of several PGQs which are organized in a hierarchical architecture. Therein, the PGQs are characterized by $PGQ_i = (L_i, F_{SLi}, F_{SSi}, F_{Mi})$, where $i=1, \dots, m$ indicates the depth index, F_{SLi} and F_{SSi} are the state following goose position influenced by the LGP of the lower layer PGQ_{*i*+1} and LGP of other PGQs, respectively. Thus, for each PGQ, we have:

$$\begin{aligned} L_i &= f_i(F_{SLi}, F_{SSi}, F_{Mi}) \\ F_{SLi} &= L_{i+1} \\ F_{SSi} &= \hat{L} \\ F_{SLiL} &\leq F_{SLi} \leq F_{SLiU} \\ F_{MiL} &\leq F_{Mi} \leq F_{MiU} \end{aligned} \quad (3)$$

where $\hat{L}$ is the LGP of other PGQs except L_{i+1} .

In order to keep the structure consistent with the actual chemical plant, F_{SSi} is deemed as the measurements of local PGQ, while $F_{SLi} = L_{i+1}$ present the lower and upper PGQ relationship, i.e., the F_{SL} of an upper PGQ may serve as the L of the next-neighbored lower PGQ in terms of increased depth index.

Figure 3 shows the cohesive graph of a multi-layer PGQ according to Eq. (3), where dash circle is used for grouping the individual PGQs.

Specifically, the economic objective function of a chemical plant optimization problem can be expressed in terms of direct related process state variables and manipulated variables. Accordingly, a concept about the

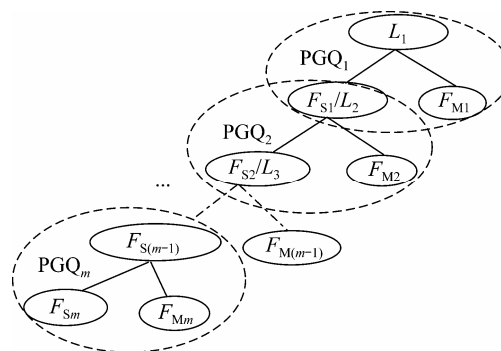


Figure 3 A multi-layer PGQ

objectives of a multi-layer PGQ is presented as follows.

Definition 4 PGQ-Objective

A PGQ-Objective is equivalent to an economic objective function of a chemical plant, characterized by

$$P = \min \varphi(P_{S1}, P_{S2}, \dots, P_{Sj}, \dots, P_{Sn}, P_M) \quad (4)$$

where, P_{Sj} ($j=1, 2, \dots, n$) and P_M are process state variables and manipulated variables, respectively. Referring back to definition 1, P_{Sj} and P_M could be similarly considered as LGP and MFGP of a PGQ, respectively. The graphical descriptions of a PGQ-Objective are shown in Fig. 4. Process state variables P_{Sj} connect the PGQ-Objective and multi-layer PGQ. Manipulated variables P_M are the manipulated variables appear in PGQ-Objective and may be coupling with other F_M in multi-layer PGQ.

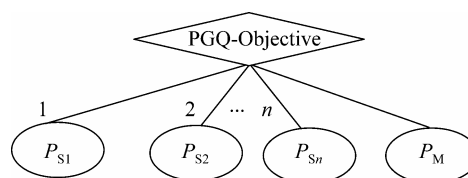


Figure 4 A PGQ (process goose queue)-Objective

Based on PGQ-Objective and multi-layer PGQ structures, the PGQ formulation for RTO is consequently described in Fig. 5.

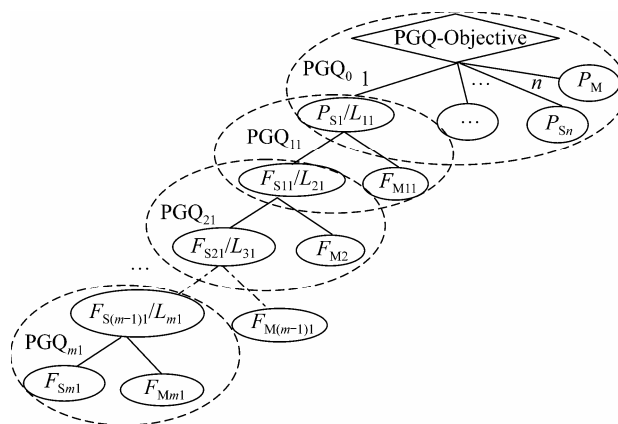


Figure 5 PGQ formulation for RTO

3.2 Implementing procedures

Uncertain disturbances may lead to deterioration of process economic performances. Therefore, the operational unit in which disturbances occur is called Ill-PGQ. Based on PGQ metrics, the implementing procedures are suggested to launch the chemical plant RTO starting with Ill-PGQ.

Step 1 PGQ follow-up

Based on the relations among LGP, SFGP and MFGP described in Fig. 5, PGQ follow-up approaches start off with the upper layer of the Ill-PGQ (PGQ_{gj}). The optimization problem behind PGQ follow-up approaches is formulated by Eq. (5) derived from Rule 1, in which the previous optimum value of PGQ_{ij} is followed and tracked by adjusting F_{Mij} , while the upper PGQ, PGQ_{(i-1)j}, would regard L_{ij} as its SFGP.

$$\begin{aligned} \min \sum_{i=g}^1 \sigma_{ij} &= \min_{F_{Mij}} \sum_{i=g}^1 (L_{ij}^* - L_{ij})^2 \\ \text{s.t. } L_{ij} &= f_{ij}(F_{SLij}, F_{SSij}, F_{Mij}) \\ F_{SLij} &= L_{(i+1)j} \\ F_{SSij} &= \hat{L} \\ L_{ijL} &\leq L_{ij} \leq L_{ijU} \\ F_{MijL} &\leq F_{Mij} \leq F_{MijU} \end{aligned} \quad (5)$$

where L_{ij}^* is the optimal position of LGP in previous optimum formation, which serves as the objective in the PGQ follow-up period.

Step 2 PGQ-Objective achievement

Based on metrics of PGQ-Objective and multi-layer PGQ, the process state variables involved in PGQ-Objective can be substituted by all LGPs with depth index 1. Thereafter, the optimum value of PGQ-Objective, P^* , can be achieved by applying Rule 1, i.e., solving the following optimization problem:

$$\begin{aligned} \min \sigma_0^2 &= \min_{P_M} (P^* - P)^2 \\ \text{s.t. } P &= \min \varphi(P_{S1}, P_{S2}, \dots, P_{Sn}, P_M) \\ L_{1j} &= P_{Sj} \\ P_{MjL} &\leq P_{Mj} \leq P_{MjU} \end{aligned} \quad (6)$$

3.3 Algorithms

According to fundamental description of the PGQ, chemical plant RTO is equivalent to implementing Rule 1 (SFGP driven adjustment rule) in the corresponding multi-layer PGQ and PGQ-Objective.

As the measurements of PGQ_i, F_{SSi} is time-varying. Conventional RTO algorithm cannot be implemented because of the failure in reaching steady-state. However, referring to RTE [15] strategy, the dynamic process of F_{SSi} can be divided into several time intervals, during which F_{SSi} is deemed as a constant. Assuming that the algorithm implementing recycle

time is equal to one time interval, Rule 1 (SFGP driven adjustment rule) is implemented to achieve the optimal PGQ-objective in sequence in the time interval. After k optimization calculations, continuous improvements of manipulated variables [$F_{Mij1}, F_{Mij2}, \dots, F_{Mij,k}, \dots, F_{Mij,N}$] are achieved.

In Eq. (5), Inequality constraints can be deleted by putting the variables within the boundary values during iteration. The first equality constraint is introduced into objective, with the result as followed:

$$\begin{aligned} \min \sum_{i=g}^1 \sigma_{ij} &= \min_{F_{Mij}} \sum_{i=g}^1 [L_{ij}^* - f_{ij}(F_{SLij}, F_{SSij}, F_{Mij})]^2 \\ \text{s.t. } F_{SLij} &= L_{(i+1)j} \\ F_{SSij} &= \hat{L} \end{aligned} \quad (7)$$

At time k , assume that an LGP_i of PGQ_i at $\overline{L_{ij,k}} = f_{ij,k}(\overline{F_{SLij,k}}, \overline{F_{SSij,k}}, \overline{F_{Mij,k}})$ has an estimate of the optimum position value $L_{ij,k} = f_{ij,k}(F_{SLij,k}, F_{SSij,k}, F_{Mij,k})$. According to Taylor expansion in first order, we can approximate:

$$\begin{aligned} f_{ij,k}(F_{SLij,k}, F_{SSij,k}, F_{Mij,k}) &= \\ f_{ij,k}(\overline{F_{SLij,k}}, \overline{F_{SSij,k}}, \overline{F_{Mij,k}}) &+ \\ \frac{\partial f}{\partial F_{Mij,k}} [F_{Mij,k} - \overline{F_{Mij,k}}] &+ v_{ij,k} \end{aligned} \quad (8)$$

where v_{ij} is the Taylor remainder.

Thus, if we specify

$$\begin{aligned} d_{ij}(k) &= f_{ij,k}(F_{SLij,k}, F_{SSij,k}, F_{Mij,k}) - \\ f_{ij,k}(\overline{F_{SLij,k}}, \overline{F_{SSij,k}}, \overline{F_{Mij,k}}) &+ \\ \frac{\partial f}{\partial F_{Mij,k}} \bigg|_{F_{Mij,k}=\overline{F_{Mij,k}}} &\overline{F_{Mij,k}} + v_{ij,k} \end{aligned} \quad (9)$$

$$\boldsymbol{\omega}_{ij,k} = [F_{Mij,k}]^T \quad (10)$$

$$\boldsymbol{u}_{ij,k} = \left[\frac{\partial f}{\partial F_{Mij,k}} \bigg|_{F_{Mij,k}=\overline{F_{Mij,k}}} \right] \quad (11)$$

The initial value of $\overline{F_{Mij,k}}$ at time k can be obtained from the previous estimate $\boldsymbol{\omega}_{k-1}$, i.e.

$$[\overline{F_{Mij,k}}]^T = \boldsymbol{\omega}_{ij,k-1} \quad (12)$$

The initial value of a PGQ, $\overline{F_{SLij,k}}$ and $\overline{F_{SSij,k}}$ at time k , can be obtained from the previous estimate $\boldsymbol{\omega}_{k-1}$, i.e.

$$\begin{aligned} \overline{F_{SLij,k}} &= L_{(i+1)j,(k-1)} = f_{(i+1)j,(k-1)} [F_{SL(i+1)j,(k-1)}, \\ &F_{SS(i+1)j,(k-1)}, F_{M(i+1)j,(k-1)}] \end{aligned} \quad (13)$$

$$\overline{F_{SSij,k}} = \hat{L}_{(k-1)} = f_{(k-1)}[F_{SS,(k-1)}, F_{M,(k-1)}] \quad (14)$$

The estimate of the LGP_i optimum position, $L_{ij,k} = f_{ij,k}(F_{SLij,k}, F_{SSij,k}, F_{Mij,k})$, can be deemed as the stepped objective and marked as $L_{ij,k}^*$. Therefore, the optimization statement of Eq. (5) turns out to be:

$$\min_{F_M} \sigma_{ij} = \min [d_{ij}(k) - \mathbf{u}_{ij,k} \boldsymbol{\omega}_{ij,k}]^2 \quad (15)$$

The optimum value of Eq. (15) can be achieved by:

$$\boldsymbol{\omega}_{ij,k} = \boldsymbol{\omega}_{ij,k-1} + \alpha \mathbf{u}_{ij,k}^\times [d_{ij}(k) - \mathbf{u}_{ij,k} \boldsymbol{\omega}_{ij,k-1}] \quad (16)$$

where α is the step length, $\times$ denotes conjugate transposition.

To study the convergence performance, Eq. (16) is expressed as

$$\boldsymbol{\omega}_k = F(\boldsymbol{\omega}_{k-1}) \quad (17)$$

The convergence performance can be measured by Lyapunov exponent:

$$\lambda = \lim_{\omega \rightarrow \infty} \frac{1}{k} \sum_{i=0}^{k-1} \ln \left| \frac{dF(\boldsymbol{\omega})}{d\boldsymbol{\omega}} \right| \quad (18)$$

If $\lambda < 0$, Eq. (16) converges, and otherwise, Eq. (16) diverges

For Eqs. (17) and (18) we have:

$$\frac{dF(\boldsymbol{\omega})}{d\boldsymbol{\omega}} = 1 - \alpha \mathbf{u}^\times \mathbf{u} \quad (19)$$

Therefore, if $|1 - \alpha \mathbf{u}^\times \mathbf{u}| < 1$ then $\lambda < 0$ and Eq. (16) converges consequently, and otherwise, Eq. (16) diverges.

Through observing the values of $\mathbf{u}^\times \mathbf{u}$ and adjusting α to fit $0 < \alpha \mathbf{u}^\times \mathbf{u} < 2$, convergence can be available.

The coupling variables $\boldsymbol{\omega} = [F_M]$ involved in a multi-layer PGQ will be affected by their neighbors. We adopt the following equations:

$$\begin{cases} \boldsymbol{\psi}_{ij,k-1} = \sum_{l \in N_i} b_{ij,l} \boldsymbol{\omega}_{l,k-1} \\ \boldsymbol{\omega}_{ij,k} = \boldsymbol{\psi}_{ij,k-1} + \alpha \mathbf{u}_{ij,k}^\times [d_{ij}(k) - \mathbf{u}_{ij,k} \boldsymbol{\psi}_{ij,k-1}] \end{cases} \quad (20)$$

The first and second equations of Eq. (20) are known as the PGQ adaptation and combination updates, respectively. $b_{ij,l}$ is considered as

$$b_{ij,l} = 0 \text{ if } l \notin M_i \times N_j \quad (21)$$

The actual solution error σ_{ij} is given by:

$$\sum_{i=1}^m \sum_{j=1}^n \sigma_{ij}^2 \leq \delta \quad (22)$$

where δ is the given error limit.

Now, the general steps of PGQ optimization algorithms are presented as follows.

Step 1 According to Eq. (20), every PGQ_{ij} adapts its current estimate $\boldsymbol{\omega}_{ij} = [F_{Mij}]$ using its individual measurements $\{L_{ij,k}^*, u_{ij,k}\}$ available at time k to obtain $\boldsymbol{\psi}_{ij,k}$. All PGQs exchange their pre-estimates $\boldsymbol{\psi}_{ij,k-1}$ with their neighbors. Every node combines the pre-estimates to obtain the new estimate $\boldsymbol{\omega}_{ij,k}$.

Step 2 The obtained $L_{ij,k}$ will server as SFGP of upper layer PGQ_{i-1} according to Eq. (13).

Step 3 Making sure that $L_{1j,k} = P_{Sj,k}$, optimize PGQ-Objective similarly using Eqs. (9)–(16) and (20) to obtain P_M .

Step 4 If a stopping criterion (22) is met, then terminate, otherwise go back to Step 1.

4 A CASE STUDY

Let's consider an exemplary chemical plant consisting of a reactor and a distillation column in an interconnected structure as shown in Fig. 6 [16, 17]. An irreversible first order reaction occurs in the continuous stirred tank reactor (CSTR). The reaction rate (γ) is a function of temperature described by Arrhenius expression. In response to the exothermic reaction, the temperature of reactor (T_r) is maintained by manipulating cooling water flow rate. Some of the reactant A

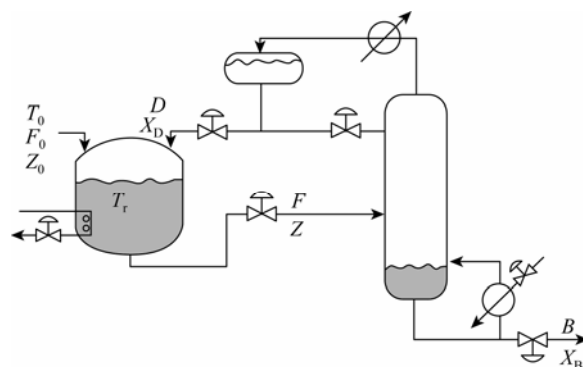


Figure 6 A reactor/separators process with recycle

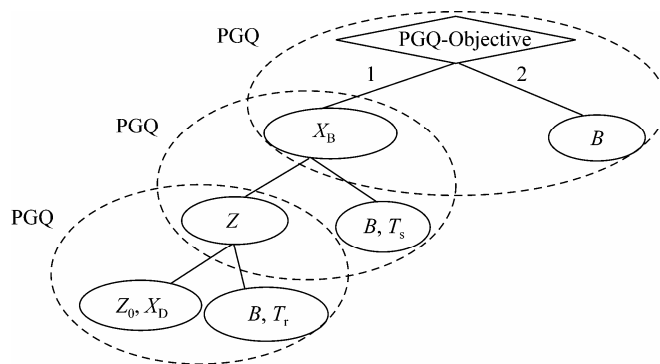


Figure 7 PGQ formulation for RTO of the exemplary chemical plant

is consumed in the CSTR, and a mixture of A and B is fed into the distillation column operated at temperature (T_s), while the product B is recycled back into the CSTR. To meet mass balance, we have:

$$\begin{aligned} \text{reactor: } F_0 + D &= F \\ F_0 Z_0 + DX_D &= FZ + V_R \gamma Z \\ \gamma &= \gamma_0 \exp\left(-\frac{E}{R_0 T_r}\right) \\ \text{column: } F &= D + B \\ FZ &= DX_D + BX_B \\ \left[\exp\left(Ai + \frac{Bi}{Ci + T_s}\right) X_B\right] / p_s &= X_D \\ \text{overall: } F_0 &= B \end{aligned} \quad (23)$$

where E and R_0 are parameters of the reactor. Ai , Bi and Ci are Antoine constants of the column.

The optimization objective is characterized by:

$$P = \min(1 - X_B)B \quad (24)$$

The manipulated and state variables are $[B, T_s, T_r]$ and $[X_B, Z, Z_0, X_D]$, respectively, and therefore, the F_{SLi} , F_{SSi} and F_{Mi} are $[X_B, Z, Z_0]$, $[X_D]$ and $[B, T_s, T_r]$, respectively. It is practical that the change of fresh feed composition (Z_0) invokes deterioration of the objective values. The corresponding PGQ formulation for RTO can be described in Fig. 7 where PGQ₂ is marked as Ill-PGQs. Optimization steps are triggered after the Ill-PGQ is detected, tracking and coordinating each individual PGQ. The objective value of PGQ can be referred elsewhere [18].

As a summary, the implementing procedures are listed as follows.

(1) PGQ₂ follow-up

Referring to the reactor mass balance in Eq. (23), the mathematical model of PGQ₂ is obtained as Eq. (25), since the Ill-PGQ, PGQ₂ tries to bring $L_2 = [Z]$ back to its previous operating points. Meantime, PGQ₂ utilizes real-time measurements, adapting and exchanging their information to obtain a new estimate of $[B, T_r]$. The resultant $L_2 = [Z]$ will server as SFGP of PGQ₁.

$$Z = \frac{F_0 Z_0 + DX_D}{F + V_R \gamma} = \frac{BZ_0 + DX_D}{F + V_R \gamma_0 \exp\left(-\frac{E}{R_0 T_r}\right)} \quad (25)$$

(2) PGQ₁ follow-up

Referring to the column mass balance in Eq. (23), the mathematical model of PGQ₁ is obtained as Eq. (26). PGQ₁ obtains a new SFGP from $L_2 = [Z]$ in PGQ₂. The new estimate of T_s is obtained by adapting and exchanging their information. The resultant X_B will server as SFGP of PGQ₀.

$$X_B = \frac{FZp_s}{D \exp\left(Ai + \frac{Bi}{Ci + T_s}\right) + Bp_s} \quad (26)$$

(3) PGQ-Objective (PGQ₀) achievement

PGQ-Objective gets SFGP from X_B achieved by PGQ₁, and therefore, obtains PGQ-Objective achievement by adapting and exchanging $P_M = [B]$.

Results of applying PGQ strategies in PGQ₂, PGQ₁ and PGQ₀ are shown in Figs. 8 (a), (b) and (c), respectively. Finally, $[B, T_s, T_r] = [468, 687, 616]$ is achieved with the objective value of 4.49.

Performance comparisons are carried out among PGQ, Multidisciplinary Design Optimization (MDO) and fmincon which is a function in Matlab with SQP or IPM method. The results are listed in Table 1. It is obvious that the PGQ method used the least elapsed time accounts for the superior performance.

Table 1 Performance comparison

Methods	Elapsed time/s
PGQ	1.236088
MDO	12.113617
fmincon	1.805469

5 CONCLUSIONS

Distinguished features associated with the PGQ based RTO methodologies could be revealed from the following manifestations.

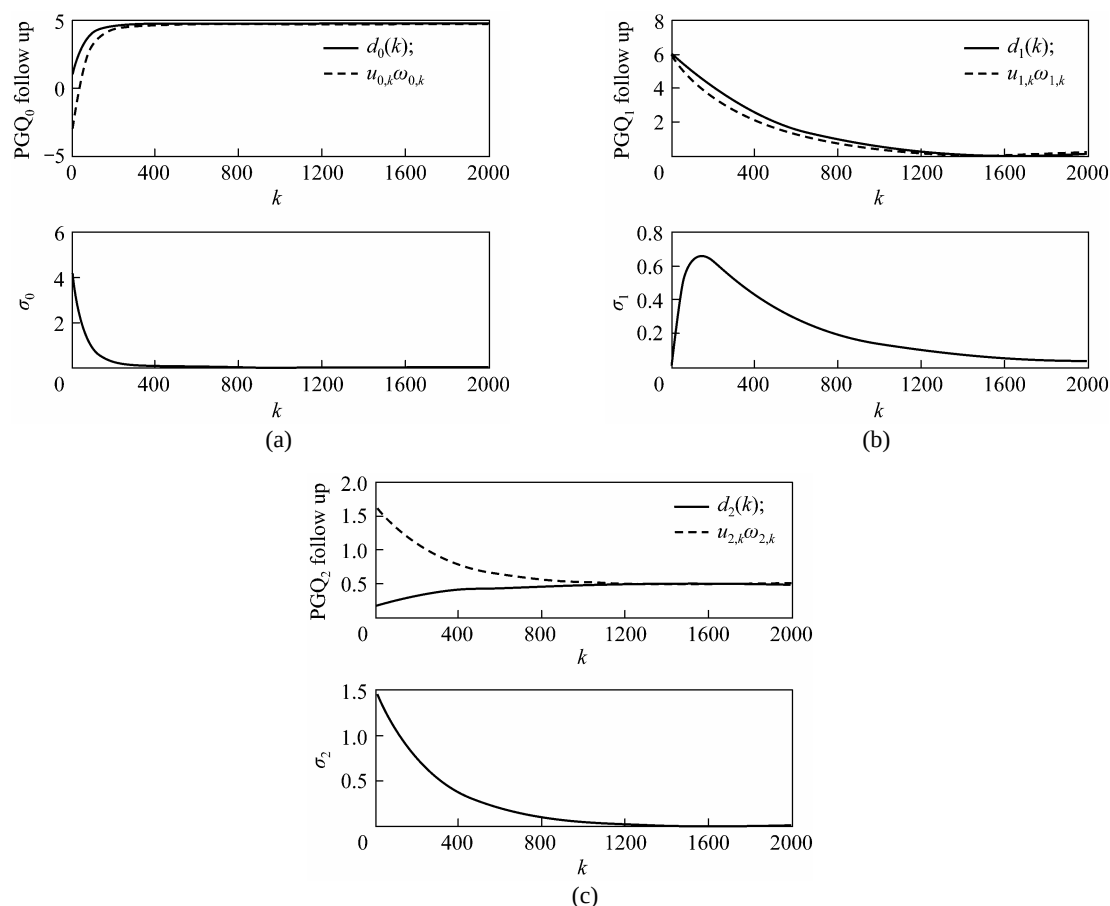


Figure 8 Results of applying PGQ algorithm in (a) PGQ₀, (b) PGQ₁ and (c) PGQ₂

(1) In contrast to conventional RTO, which usually optimizes a complex objective function involving enormous manipulated variables, PGQ-RTO decomposes the optimization problem into several PGQ follow-up implementations, leading to considerable computational simplicity.

(2) PGQ methodologies are recognized to utilize more real-time measurements which are beneficial for chemical plant real-time optimization.

In spite of our efforts on demonstrating the feasibility and validity of the contribution through a case study, the convergence issues of the PGQ methodology still remain to be investigated mathematically in future. In particular, it is estimated that tradeoffs between convergence speeds and performance might be available, which is expected to promote our research work more attractive.

NOMENCLATURE

A_i, B_i, C_i	Antoine constants of column
B	bottoms flow rate from column
D	distillate flow rate from column
E	activation energy of the reactor
F	reactor effluent flow rate
F_M	the manipulated following goose position
F_S	the state following goose position

F_{SLi}	the state following goose position influenced by L_{i+1}
F_{SSi}	the state following goose position influenced by $\hat{L}$
F_0	fresh feed flow rate to reactor
f	the relationship among LGP, SFGP and MFGP
f_0	the upwash function in physical flying goose queue
g	steady-state relationship function
k	time
L	the leading goose position
L_{i+1}	the LGP of the lower layer PGQ _{$i+1$}
$\hat{L}$	the LGP of other PGQs except L_{i+1}
L_{ij}^*	the optimal position of LGP in previous optimum formation
P^*	optimum value of PGQ-Objective,
P_M	process manipulated variables in objective expression
P_{Sj}	process state variable in objective expression
p_s	pressure of distillation column
R_0	perfect gas law constant of the reactor
S	vector of input variables
T_r	temperature of reactor
T_s	temperature of distillation column
V_R	reactor holdup
X	vector of manipulated variables
X_B	bottoms composition
X_D	distillate composition
x	horizontal coordinate of physical flying goose
Y	vector of output variables
y	vertical coordinate of physical flying goose
Z	reactor composition
Z_0	fresh feed composition to reactor
α	step length

γ	reaction rate
δ	the given error limit
σ_{ij}	actual solution error
ϕ	empty set

Superscripts

$\times$	conjugate transposition
$*$	the optimum value

Subscripts

i	the depth index of multi-layer PGQ
j	the breadth index of multi-layer PGQ
L	lower bound limit
U	upper bound limit

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