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OPTIMAL CONTROL OF PARALLEL BATCH REACTORS

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Abstract. In this paper joint control and optimization problems of parallel processing batch reactors are considered. The specific problem addressed is the on-line scheduling of oxidation reactors in Dymethyl terephthalate (DMT) producing plant. Three level hierarchical control system is proposed to coordinates off-line optimization of batch profiles and schedules with on-line multilevel control. A reactive layered multifunctional scheduler is developed to react adequately to the batch processes variability as well as to the operations in the downstream and upstream stages of the whole plant. Results of computer simulation tests as well as some partially applications are presented.

Key Words. Batch process, control, optimization, oxidation, reactor, scheduling.

1. INTRODUCTION

Optimal control of parallel batch reactors continue to be object of intensive investigations [2,5,7,8], but a small part of achieved results still find real application [5,7,8]. Formal methods for formation of non-contradictory schedules of industrial systems are given in [2,5,8]. The choice of different variants of control variables is studied in [5] where has been shown that combination of formal and heuristic methods can be very effective because the volume of calculations is highly reduced. The influence of the variability of the characteristics of individual batch reactors is emphasized in [2]. The approach with using of off-line calculated reference schedules, which are later corrected in one way or another, is widely used [2,5]. The problems with maintaining of the level in the storage tanks have been studied in a number of works as a resource constraint [2,5,7] and different approaches have been suggested for their solution [5,8].

In the present paper, unlike the above mentioned contributions in which scheduling problems are mainly discussed, the optimal control of parallel batch reactors is stated as multilevel one using different optimization, control and scheduling techniques.

2. SYSTEM REPRESENTATION

In the present paper the generic methods for optimal coordinated control are applied on the oxidation stage of DMT production plant [1,4,6]. The structure scheme of it is shown on Fig.1.

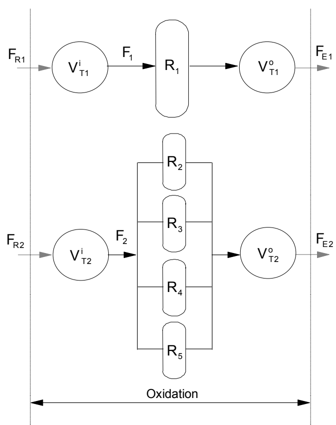


Fig.1.Structure of oxidation stage

The group of five reactors and storages connected in parallel is distributed in two production lines A and B. The process diagram of all reactors is identical and is shown in Fig.2. Technological sequence of reactors contains the following operations: (1) charging the reactors with p-Xylene (pX), working p-methyl toluate (pMT) and liquid catalyst, (2) heating the rector, (3) blowing the reactor contents with insertion air, (4) additional charging with working p-methyl toluate, and (5) emptying the reactor. After corresponding idle time a new batch cycle begins.

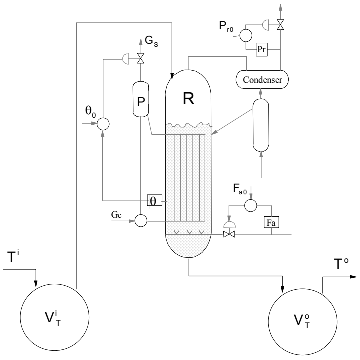


Fig.2.Scheme of oxidation reactor with input and output tanks.

Reactors operate independently but the execution of individual operations on different oxidation reactors must be coordinated. Timetable for j-th reactor includes the following time intervals (Fig.3): t_{fj} - feeding time, t_{pj} - processing time, t_{ej} - emptying time, t_{hj} - holding time, t_{dj} - dephasing time.

The batch time t_{bj} is the interval between start time and completion time

$$t_{bj} = t_{fj} + t_{pj} + t_{ej} + t_{hj} \tag{1}$$

Feeding times t_{fj} and emptying times t_{ej} have constant values, but another timetable elements should be determined by scheduler.

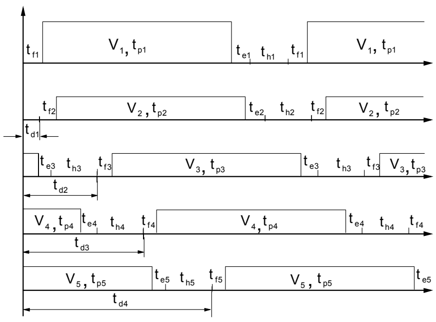


Fig.3.Dephased cyclic processing of the oxidators.

3. PROBLEM FORMULATION

The optimization of parallel processing batch reactors is studied in the paper in two aspects:

a) optimization of processes in a single reactor;

b) optimization of parallel batch reactors.

The optimization problem for each individual reactor is solved for minimal processing time for a given batch size V, charging ratio γ and p-methyl toluate concentration(C_{PT}) in the inlet flow:

$$t_P = t_P(V, \gamma, C_{PT}) \rightarrow \min \tag{2}$$

As the optimization of charging ratio γ is a problem of the plant wide and deviation of p-methyl toluate concentration is a result of whole plant operation, for the optimization problem (2) γ and C_{PT} should be considered as a given parameters. Therefore after solving the optimization task (2) the processing time t_P depends only on batch size V:

$$t_P = t_P(V, \gamma^0, C_{PT}^0) = t_P(V) \tag{3}$$

The profit rate has been assumed as a suitable economic criterion, defined as follows:

$$P = \frac{R - (I + O)}{t_f + t_P + t_e + t_h} \tag{4}$$

where R, I and O are sales and steam revenue, inventory charges and operation costs correspondingly. Taking into account the relation (3), the profit rate of the separate oxidation reactor is a function of the batch size Vj and the idle time t_{hj}

$$P_j = P_j(V_j, t_{hj}) \tag{5}$$

The relation (5) is valid for the given γ^0 and C_{PT}^0. If they latter change the profit P_j changes as well. The p-methyl toluate concentration(C_{PT}) is analyzed rather infrequently [1] so the corrections in P_j can be done only periodically. Because of this and also due to intrinsic process disturbances relation (3) can fluctuate in certain boundaries and impose changes in priory envisaged processing time t_{Pj}.

The anticipated production rate F_j for given γ^0 and C_{PT}^0 is defined in a similar way as:

$$F_j = F_j(V, t_{hj}) \tag{6}$$

The optimization of the group of parallel processing oxidation batch reactors is realized by the supervisory control level for performance-based scheduling objective criterion - profit maximization under numerous constraints:

$$P = \sum P_j(V_j, t_{hj}) \rightarrow \max \quad (j = 1, 2, \dots, n_j) \tag{7}$$

subject to

$$h_l(V_j, t_{hj}, \mathbf{q}) = 0 \quad (l = \overline{1, m_l}) \tag{8}$$

$$g_r(V_j, t_{hj}, \mathbf{q}) > 0 \quad (r = \overline{1, m_r}) \tag{9}$$

Constraints (9) depend not only on intergroup variables $V_j, t_{hj}\ (j = \overline{1,5})$, but also on variables external for the group of parallel reactors, represented by vector $\mathbf{q}$ as follows: input and output flow rate, charging ratio γ^0 and concentration C^0_{PT}. Part of constraints (9) guarantee the location of the input and output storage tank levels (Fig.1, Fig.2) between the set upper and lower limits. This necessitates the introduction of a third optimization vector - dephasing times t_d. If the operating conditions of the upstream and/or downstream stages are changed the existing schedule must be adjusted or re-optimized.

4. CONTROL STRUCTURE

A three-level hierarchical system for optimal coordinated control of parallel batch oxidation reactors is shown in Fig.4. It involves:

- *First level* (L1), in which are present PID controllers for stabilizing the set reactor temperature θ^0 and air flow rate F^0_a as well as PLC for the reactor filling, starting, recharging and emptying.
- *Second level* (L2), in which the following tasks are performed:

  - Off-line model-based maximal speed optimization for defining of an optimal batch profile for each reactor;

  - Reactor charging and recharging.

  - Model-based inferring of the reactor process state by reconstruction of specially formed "acidity number" χ [1].

  - On-line re-optimization and sequenced correction of the predefined optimal set-points for first level controllers θ^0 and F^0.
- *Third level* (L3) where the following tasks are running:

  -Off-line creation of the reference production rates F^0_j for each parallel reactor as well as the maximal profit rate P^0 for whole group of reactors.

  -Off-line construction of optimal process schedule for each reactor, i.e. the third level control variables - batch size V_j, holding time t_{hj} and dephasing time t_{dj}.

  -On-line correction of all deviations from optimal scheduling by re-scheduling.

  -On-line monitoring and control of the input and output tank's levels.

  -Periodically off-line estimation of the p-methyl toluate concentration (C_{PT}) and charging ratio γ and restarting corresponding re-optimization procedure if violated.

Control structure could be considered as a multicascade one, where the level's control loops are temporarily distinguished (Fig.4). The typical transfer times for corresponding levels are 30 min, 14 h and 7 days. Therefore the higher level influence the lower level in static way and a temporal decomposition is reasonable.

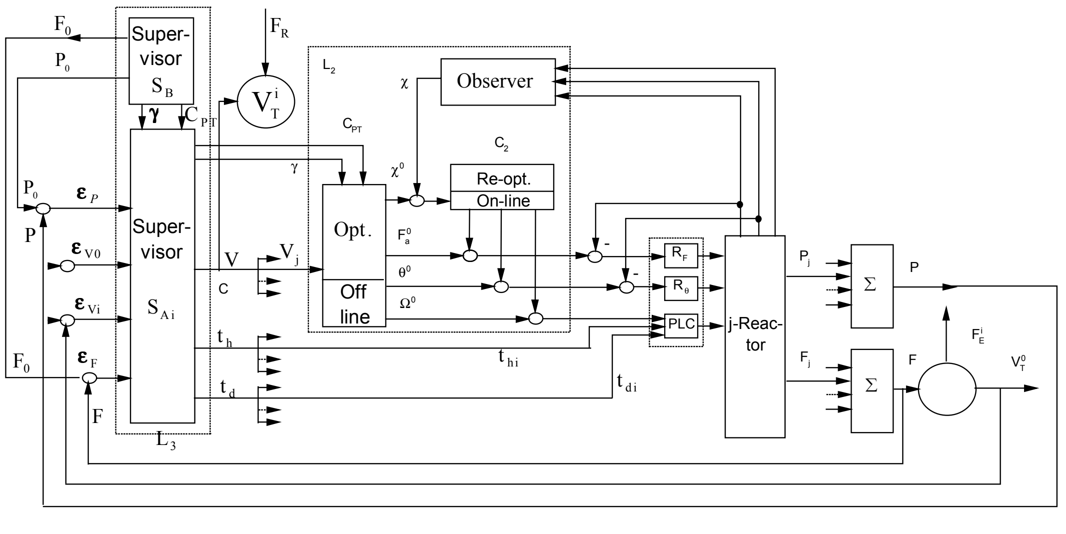


Fig. 4. Scheme of parallel batch reactors control system

5. OPTIMAL CONTROL OF SEPARATE REACTOR

As it was reported in [1], the main oxidation reactor control problem consists is the lack of direct measurements of key process variables. Because of that a model based control is implemented as a main control strategy.

5.1. Open Loop Inference Control

The off-line optimal batch profile is determined in the following sequence:

- Upgrading the complete mathematical model of the oxidation process, presented in a state space form [1]

$$\frac{d\mathbf{X}}{dt} = f(\mathbf{X}(t), \mathbf{U}(t), \alpha, \beta) \quad \mathbf{X}(0) = \mathbf{X}_0 \qquad (10)$$

where $\mathbf{X}(t)$ is a generalized reactor state vector, including the chemical concentrations of reagents, temperature and pressure in batch contents; $\mathbf{U}(t)$ is a vector of control variables, involving the air flow rate, steam generated flow rate and parameters of reactor recharging; α, β are vectors of coefficients; $\mathbf{X}_0$ is a vector of the initial conditions.

- Using NLP optimization [1, 3], the optimal control vector $\mathbf{U}^*$ is derived in order the processing time t_P to be minimized. As a result the optimal set-point's time profiles F_a^0 and θ^0 for the local controllers R_F and R_θ are received. An example for the reactor included in the production line A is presented in Fig.5b and Fig.5c.

- Forming the optimal time profile for the proposed in [1] simplified indirect indicator of batch contents state, called "acidity number" χ^0 (Fig.4). It is shown in Fig.5a.

- Generating the settings Ω^0 for the PLC operations (Fig.4).

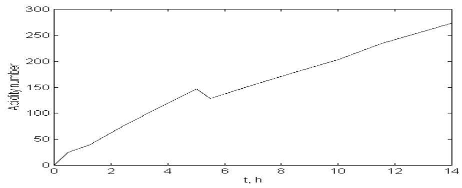
5.2. Feed Back Control

A model based observer for on-line estimation of the "acidity number" χ is carried out using a set of indirect available measurements. A re-optimization procedure is started 3-4 times during the batch processing in order to realize on-line correction of predetermined local controller's set points - air flow rate F_a^0, reactor temperature θ^0 and discrete operation schedule Ω^0.

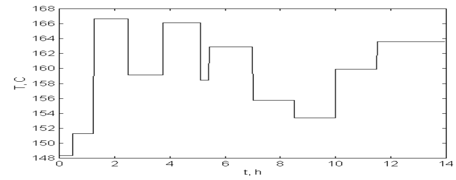
5.3. Resulting Relationships

Using the NLP based optimization a set of resulting relationships are received, namely:

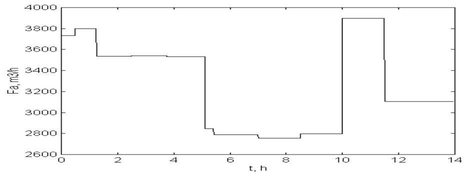
- The processing time t_P vs. batch size V, according the equation (3). They are presented in Fig. 6 in the dependence on the p-methyl toluate concentration (C_{PT}^0) (a) and the charging ratio γ^0 (b).



a)

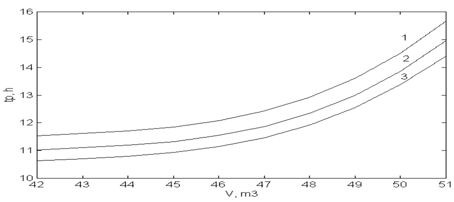


b)



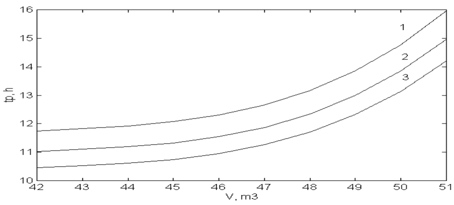
c)

Fig.5. Optimal time profiles for acidity number χ (a), temperature T_R (b) and air flow rate Fa; t - processing time.



a

$C_{PT} = 55\%$ γ =0.45(1), γ =0.60(2), γ =0.75(3)



b

γ =0.60

$C_{PT} = 45\%$ (1) $C_{PT} = 55\%$ (2) $C_{PT} = 65\%$ (3)

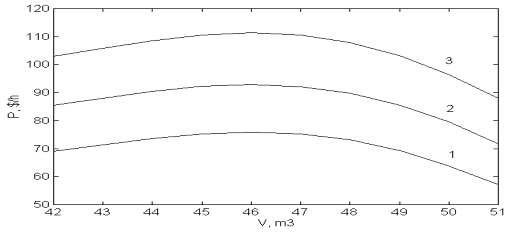
Fig.6. Processing time as a function of the batch size.

- The profit rate P vs. batch size V, corresponding to the equation (4). They are shown in Fig.7 in dependence on C_{PT}^0 (a) and γ^0 (b).

- The profit rate P as a function of the batch size V and the holding time t_h (Fig.8)

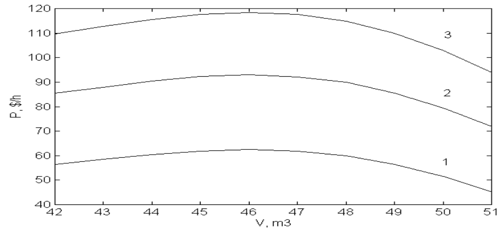
- The processing rate F vs. the batch size V and the holding time t_h. It is similar on the relationship presented in Fig.8.

All received relationships are used in the off-line scheduling procedure generation.



a

$C_{PT} = 55\%$ γ =0.45(1), γ =0.60(2), γ =0.75(3)



b

γ =0.60

$C_{PT} = 45\%$ (1) $C_{PT} = 55\%$ (2) $C_{PT} = 65\%$ (3)

Fig.7.Profit rate as a function of batch size

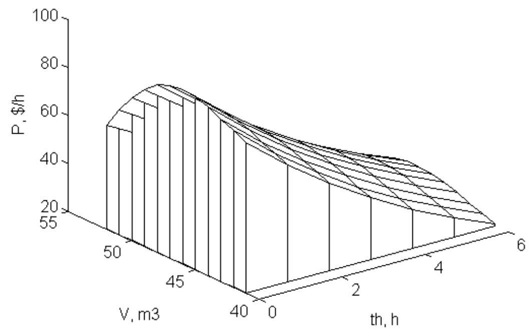


Fig.8.Profit rate as a function of V and t_h.

6. OPTIMAL CONTROL OF PARALLEL REACTORS

The supervisory parallel batch reactor's control system (Fig.4) is multifunctional one in order to achieve high efficiency and reliability of the oxidation stage. It is the most important in the DMT production du to the very limited possibilities to influence on the chemical composition of the leading components in the downstream units as well as because it realize about 70% of the whole line profit.

6.1. Off-line Scheduling

The aim of the off-line scheduling is to construct optimal timetables for each of the parallel processing batch reactors in the parallel production lines A and B (Fig.1) in order to maximize the all stage profit P according the equation (7) during each planing period defined from the current single product demand. Based on the equations(8) and (9) the following constraints must be satisfied:

- Equality type constraints (8):

Current production rate of oxidat F(k) to be equal to the given one F^0 received from the production planer [4]

$$F^0 = \sum_{j=1}^{5} F_j(k) \qquad (11)$$

- Inequality type constraints (9):

- Restrictions for the each reactor production rates;

$$F_j^{min} \le F_j(k) \le F_j^{max} \quad (j = 1,2,\ldots,5), \qquad (12)$$

where F_j^{min}, F_j^{max} are admissible low and high capacity of the j-th reactor.

- The current volumes of the input and output storage tanks to be between fixed low and high values

$$V_{Tj}^{min} \le V_{Tj} \le V_{Tj}^{max}, \qquad (13)$$

where $V_{Tj}(k)$, V_{Tj}^{min} and V_{Tj}^{max} are current, minimal and maximal admissible volumes of j-th input or output tank.

Two step procedure is developed to solve the optimizing problem (7):

1.Determination the technological structure (TS). TS is called each admissible combination of reactors included in the lines A and B (Fig.1) which could satisfy the requirement of the production rate (11). TS may be considered as a subset S_r of the set S of admissible technological structures {S: [1,0; 1,2; 1,2,3; 1,2,3,4; 1,2,3,4,5: 0,2; 0,2,3; 0,2,3,4; 0,2,3,4,5; 0,0]}. To find the relationships

$$S_r = S_r(F^0) = S_r(V, t_h) \;, S_r \in S \qquad (14)$$

the NLP procedure [3] is realized to solve the optimizing problem (7) with the constraints (11)-(13) in the full range of possible production rates (in the case 1.28 t/h< F_i <9.58 t/h). For the each given production rate F^0 a very limited number of admissible technological structures, satisfying the constraint (11)-(13) could be find. This eliminate the combinatorial problem and no MINLP is necessary to be used for the optimization.

2. For given: operation conditions, production rate F^0, charging ratio γ^0, p-methyl toluate concentration (C_{PT}^0) and fixed possible TS_l, the NLP procedure is executed in order to find the maximal profit rate P_l for each l-th TS as well as corresponding optimal vectors of batch sizes V^l and holding times t_h^l. The comparison between scanned

TS' determines uniquely the best TS and corresponding control vectors V^* and t_h^* for which the stage profit rate is greatest.

Preliminary analysis for variety of operation conditions (F^0, γ^0, C_{PT}) can be accomplished to decide if holding time is needed to satisfy constraints(13). In this way the computing time of optimization procedure could be reduced additionally.

The constraints (13) are satisfied using the additional degree of freedom - initial dephasing time t_{di}. The optimization of t_{di} is a result of decision the problem

$$J = \min(\max|\overline{V}_{Tj} - V_{Tj}(k)|) \qquad (15)$$

where $\overline{V}_{Tj}$, $V_{Tj}(k)$ are the average and current volume in the j-th tank (Fig.9). If batch sizes V_i are given, the criterion (16) depends only on dephasing times t_{dj} and vector $\mathbf{q}$ according the equations (8) and (9). NLP procedure gives the optimal values of reactor starting times.

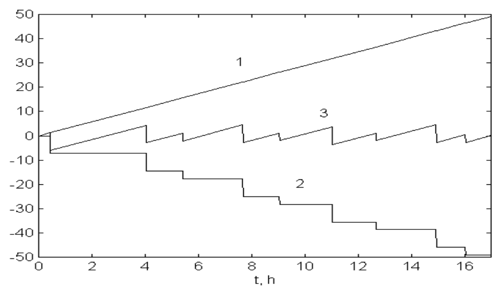


Fig.9. Volume behavior of the input tanker V_{T2}^i

6.2.Reactive Scheduling

The proposed scheduler reacts to the errors $\Delta P^0, \Delta F^0, \Delta L_j^i, \Delta L_j^0$ and forms relevant control actions $\Delta V_i, \Delta t_{hi}, \Delta t_{di}$ (Fig.5). The algorithm of this reactive scheduler is specific form of MBPC [7]. It realize the next steps:

1. Analysis of supervisor's input signals and formation of corresponding errors.
2. Comparison of the old and new values of the charging ratio γ and the p-methyl toluate concentration (C_{PT}) and as a result additional errors $\Delta\gamma$ and ΔC_{PT} formation.
3. If some of the above errors exceed given threshold the scheduling procedure described above is restarted.
4. New schedule will be executed up to the next appearing of input error.

In contrast of [2,5] where the off-line constructed schedule is corrected we implement full re-optimization, du to the modest computational efforts. For PC with 166 MHz the scheduling optimization take 5 min, which is very small according to the time scheduling horizon (7 days).

7. CONCLUSIONS

A hierarchical control system for economical optimization of parallel processing batch reactors is proposed using joint NLP and MBPC approaches. Multifunctional supervisor is developed for reactive scheduling, process optimization and storage tank levels holding up in permissible bounds. Reduction of the complexity of the scheduling procedures is achieved by combination of off-line and on-line procedures as well as a relevant decomposition.

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