CHEMICAL ENGINEERING TRANSACTIONS

VOL. 70, 2018

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Timothy G. Walmsley, Petar S. Varbanov, Rongxin Su, Jiří J. Klemeš

ISBN 978-88-95608-67-9; **ISSN** 2283-9216

DOI: 10.3303/CET1870095

Dynamic Process Simulator Assisted Optimization of Operating Point Transition

Alex Kummer*, Tamás Varga

Department of Process Engineering, University of Pannonia, H-8200, Veszprém, Hungary
kummera@fmt.uni-pannon.hu

Model-based dynamic optimization is an effective tool for control and optimization of chemical processes, especially during transitions in operation. This study considers the dynamic optimization of load transitions. Poor operating point transition strategy can increase the quantity of off-spec product coming with financial loss, and also can increase the risk of malfunctions. A novel methodology for operating point transition optimization is applied to a vacuum distillation column unit in which concentration of cumene-hydroperoxide intermediate occurs. Optimization task is based on Open Platform Communication (OPC) between a commercial process simulator (Aspen HYSYS) and MATLAB. Nonlinear Optimization with Mesh Adaptive Direct Search algorithm (NOMAD) is applied to solve the task. Load of the distillation column is decreased from 100% to 90% taking into account the time of transition, amount of off-spec product and energy consumption. Different objective functions result definitely different transition strategies, therefore the right choice of this function is crucial step in this process. The results show that the proposed optimization methodology can be applied efficiently based on a complex simulator of the technology.

1. Introduction

In industrial chemical processes operating point transition can be weekly due to any change in desired product, different required load of processes or raw materials quality. During the operating point transition, the product might not meet the quality requirements, which causes financial loss, or the technology can quit from the controllable zone and a hazard situation can occur, which risks the life of process operators. A well-defined strategy on how to change operating point can help to avoid loss and decrease the risk of malfunctions during transitions. Modern chemical processes become more complex via the number of connections between the technological units, therefore the effect of any change in parameters cannot be determined with the necessary precision. Wang et al. (2017) developed a real-time optimization and control framework tested on an industrial ethylbenzene dehydrogenation process model described by Partial Differential Algebraic Equations.
Nowadays the requirements for more and more accurate simulators are already high, therefore taking into account the thermodynamic of the real system is key component in building an adequate simulator. Commercial process simulators are applied worldwide to solve problems related to an industrial technology or in research and development procedure of a none existed ones. Aspen HYSYS (or other commercial process simulators (PS)) can be applied for such a problem using a communication bridge between PS and MATLAB, which simplifies the model building part of the task. Open Platform Communication (OPC) can create a connection between Aspen HYSYS and MATLAB therefore a commercial PS based optimization can be performed.
Dynamic process simulators (DPS) should be applied to analyze the transient behavior of technologies. DPS apply mathematics and first principles (thermodynamics, transport phenomena, etc.) to make an adequate and reliable representation of industrial chemical processes. Operator Training Simulator (OTS) Market Research (2017) shows that there is an increasing demand on OTS systems in the world, which is a good basis for transition optimization. Sritharan et al. (2017) developed an adequate OTS for ethylene plant and tested for start-up, shutdown and malfunction events.
Perez et al. (2002) suggested to apply inversion-based approach to switch between operating points, where the system dynamics is inverted to find the input that exactly tracks a single output trajectory. Common problem is optimal grade transition, where the objective function is usually defined in terms of the amount of off-spec

Please cite this article as: Kummer A., Varga T., 2018, Dynamic process simulator assisted optimization of operating point transition , Chemical Engineering Transactions, 70, 565-570 DOI:10.3303/CET1870095

product, product quality specifications, grade changeover time and process safety constraints (Chatzidoukas et al., 2003). McAuley and MacGregor (1992) showed that the calculated optimal transition strategy was strongly dependent on the objective function and the presence of constraints.

Building an adequate dynamic process simulator of any technology is a complex and difficult task in itself. The transition optimization problems are mostly based on simplified simulators applied to define the optimal parameters of transition and only a few works can be found in which PS were applied in such a task. In this work we would like to show how commercial process simulators can help to solve the transition problems. The operating point transition of a vacuum distillation column of a phenol production technology is investigated, in which the concentration of cumene-hydroperoxide intermediate is realized (Schmidt, 2005). The simulator of the column is developed in Aspen HYSYS environment.

The operating point transition was defined here as a nonlinear optimization task with constraint. Nonlinear Optimization with MADS algorithm (NOMAD) algorithm was applied to solve the optimization problem and the optimization task was solved in MATLAB program (Le Digabel, 2011).

2. Case study

Phenol production from cumene takes two reactions steps. The first step is oxidation of cumene to cumene-hydroperoxide (CHP) with 25-30 % conversion, where air is bubbled through liquid cumene in oxidation reactors. Phenol comes from cleavage of CHP, but in the previous step the diluted CHP has to be concentrated. The concentration of CHP (to ~ 60 w%) is done in vacuum distillation column, where the bottom product is the concentrated CHP, and cumene comes as a distillate. The second reaction is CHP cleavage under acidic conditions to produce phenol as product and acetone as co-product in continuous tank reactor (Schmidt, 2005). The developed process simulator of vacuum distillation column is shown in Figure 1. DPS include hydrodynamics and also hydrostatic calculations which help to develop an adequate simulator of the process unit.

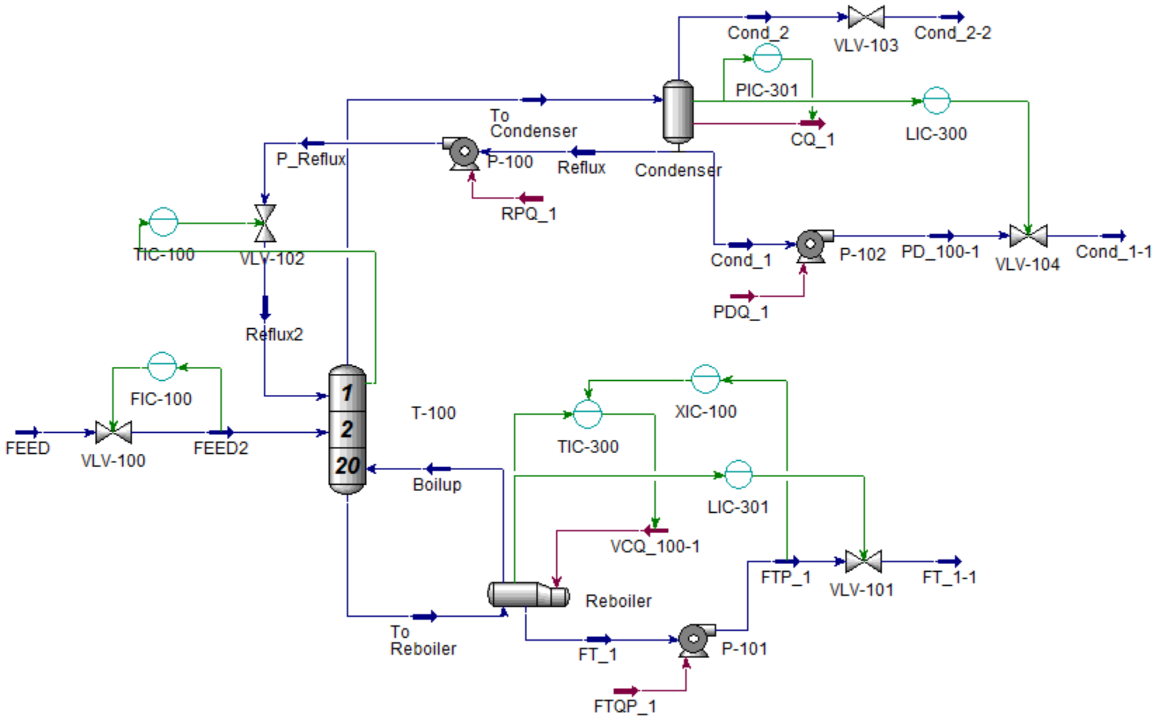

Figure 1: Process simulator of the investigated vacuum distillation column (Aspen HYSYS)

The operation of T-100 vacuum column is controlled by tuned PI controllers. FIC-100 controls the flow rate of feed cumene-CHP mixture. LIC-300 and LIC-301 controls the level in the reflux drum and reboiler by opening the outlet valve. The temperature of reboiler is controlled in cascade, where the secondary controller (slave) is TIC-300, and the primary controller (master) is XIC-100. Concentration of CHP in FTP_1 stream is measured and controlled by XIC-100. TIC-100 controls the tray temperature by reflux flow rate. The pressure of condensate tank is controlled via PIC-301 by cooling the condensate tank with cooling water.

Usually in a process simulator does not include any optimization module, or only simple optimization problems can be solved performing sensitivity analysis. However, in MATLAB there is a huge choice of efficient optimization algorithms which can be used in transition optimization. Aspen OTS Framework can create an OPC server, and can create a connection between MATLAB and Aspen HYSYS. OPC connection allows the online modification of the operating parameters, and all collected data can be efficiently analyzed in MATLAB.

3. Operating point transition

In industrial chemical processes operating point transition can be weekly task involved several risks and financial loss. Analyzing the dynamics of operating point transitions can help to decrease the amount of off-spec product and minimize the energy consumption and the required time to switch between operating points. Analyzing continuous processes with one-spec product the operating points of the plant can be defined with different load of the plant.

In this work an optimization task was performed based on the simulator of vacuum column, where the flow rate of feed was decreased (i.e. the setpoint of FIC-100) by ten percent in steps. Figure 2 shows the operating point transition, where F is the feed rate, and t is time. Searching variables in the optimization task are number of steps in feed rate during operating point transition (n), time of the specific internal step (t_x), and the internal setpoints (F_x).

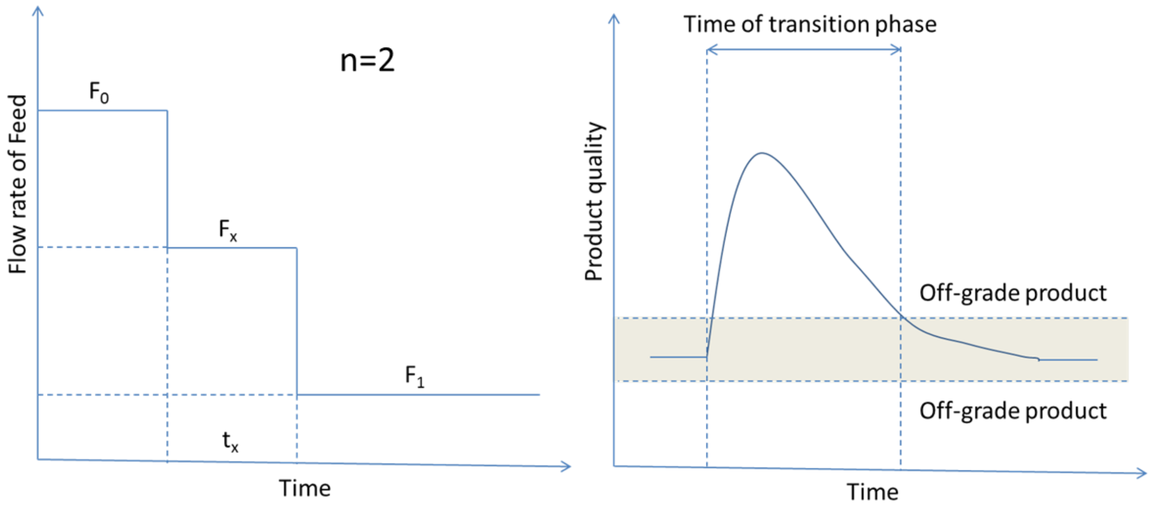

Figure 2: Operating point transition

Three different strategies for operating point transition have been performed to get reference, where the number of steps and time of internal steps were changed. Internal load setpoints were calculated and collected in Table 1 which includes the parameters of operating point transition functions and also the time of transition phase (TTP), invested energy of transition (IET), and the amount of off-grade product (OGP). The product is off-grade if the weight CHP concentration does not remain in 60±0.3% range.

The internal setpoints were calculated with eq. 1-3, where SP is setpoint, SP_{op0} is initial setpoint, $SP_{op,new}$ is the new setpoint, and p_i is the ratio off the i^{th} internal step.

$$SP_i = SP_{op0} - \sum_{i=1}^{i} p_i m \qquad (1)$$

$$m = SP_{op0} - SP_{op,new} \qquad (2)$$

$$\sum_{i=1}^{n} p_i = 1 \qquad (3)$$

Table 1: Parameters of reference operating point transitions

No.	n	t_x [min]	p_1	p_2	p_3	p_4	p_5	TTP [min]	IET [MJ]	OGP [kg]
1	1	0	1	0	0	0	0	16.62	3.32	1210
2	2	13.3	0.5	0.5	0	0	0	23.00	1.67	1737
3	5	3.33	0.2	0.2	0.2	0.2	0.2	22.70	0.68	1519

Figure 3 shows how the different strategies influence the product (CHP) concentration, flow rate of product, and the required energy. Different strategies lead to fully different transition trajectories, producing different amount of off-grade product and requiring different invested energy stream.

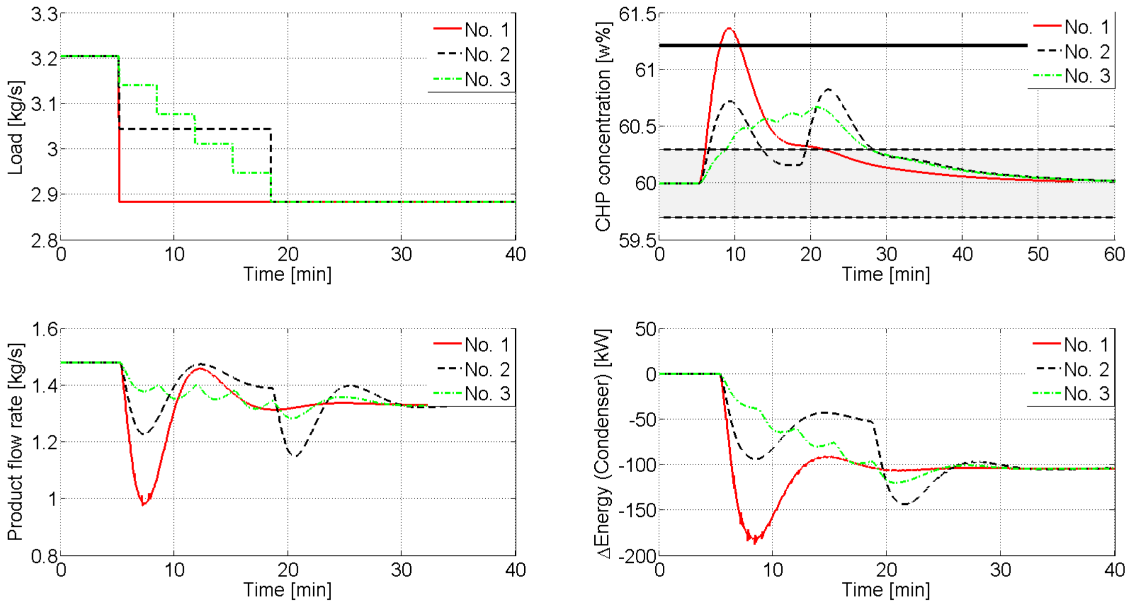

Figure 3: Different strategies of operating point transition

Objective function influences the optimal transition strategy, therefore four objective functions are applied to determine the optimal strategy. In first case (Eq(4)) the time of transition phase (TTP) was minimalized, in second case (Eq(5)) the invested energy of transition was minimalized. Invested energy flow of transition was calculated with Eq(6), where Q_i means the energy flow through condenser and reboiler, $Q_{i,0}$ means the energy flow through condenser and reboiler in steady-state of starting operating point. In the third case the amount of off-grade product was minimalized (Eq(7)), and in the fourth case the combination of first and second objective function was applied (Eq(8)).

$$of_1 = TTP \tag{4}$$

$$of_2 = \int \sum \Delta Q_i \, dt \;\; where \;\; \Delta Q_i > 0 \;\; and \; i = \{cond, reb\} \tag{5}$$

$$\Delta Q_i = Q_i - Q_{i,0} \;\; where \; i = \{cond, reb\} \tag{6}$$

$$of_3 = \int \dot{m}_{off-grade} dt \tag{7}$$

$$of_4 = TTP + \int \sum_i \Delta Q \, dt \;\; where \;\; \Delta Q_i > 0 \;\; and \; i = \{cond, reb\} \tag{8}$$

High CHP concentration can lead to accident in a cleaving reactor after the CHP concentration unit, therefore a constraint was defined in every optimization task (Eq(9)) as the maximum CHP concentration during transition cannot be higher than 61.2 w%.

$$\max(w_{CHP}) \leq 61.2\% \tag{9}$$

4. Results

The different transition strategies derived from different objective functions can be seen in Figure 4, and the optimized parameters of transition functions are collected in Table 2. Objective functions highly influence the strategy of operating point transition, therefore it is important to evaluate the choice. Optimizing the transition can save a significant amount of production time, invested energy and can decrease the amount of off-grade product. Despite of minimizing the TTP (No. 1) the optimal value of TTP is higher than the TTP from non-optimized operating point transition (Table 1), but as it can be seen in Figure 3, the safety limit of high CHP concentration was violated there. A similar tendency can be noticed in case of minimizing the amount of off-grade product (No 3.) and the first reference case. The most significant progress is achieved in case the OGP from the previously described performance indicators after the optimization procedure compared to the reference cases.

Table 2: Parameters of optimal operating point transitions considering different objective function

No.	n	t_x [min]	p_1	p_2	p_3	p_4	p_5	TTP [min]	IET [MJ]	OGP [kg]
1	2	4.17	0.87	0.13	0	0	0	17.00	2.84	1243
2	5	3.33	0.03	0.08	0.29	0.30	0.29	24.60	0.11	1313
3	3	6.64	0.17	0.09	0.74	0	0	25.20	0.82	856
4	3	2.24	0.44	0.39	0.17	0	0	17.58	1.49	1254

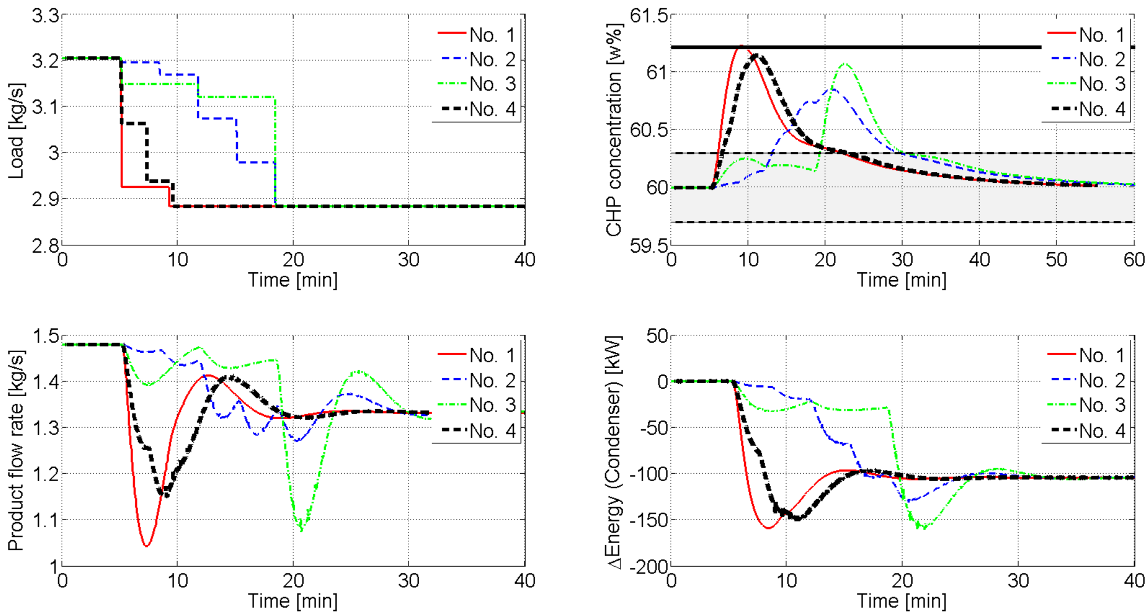

Figure 4: Optimal strategy of transition due to different objective functions

In case of a distillation column minimum energy requirement during transition means to switch between operating points as slow as possible, which is going against the minimum transition time, so the combination of this two performance indicator should be considered in optimization as it was evaluated at No. 4 task.

5. Conclusion

Operation optimization of chemical processes involves two aspects: steady-state and dynamic optimization. Steady-state optimization is necessary to perform for knowing the optimal process parameters during normal operating conditions. However, process disturbances can occur, or process conditions can change, and the

state variables will vary with time. The safety limits and constraints can be violated during transitions between optimal operating points obtained in steady-state optimization, therefore the dynamic optimization is necessary to perform to drive the process variables according to the safety limits and to evaluate achievable benefit.
In this work it has been shown that operating point transition optimization problem can be efficiently solved using a commercial process simulator. The dynamic process simulator of cumene-hydroperoxide concentration was developed in Aspen HYSYS. NOMAD global extremum search algorithm implemented in MATLAB was used to solve the nonlinear optimization task. A data link was established between MATLAB and Aspen HYSYS, which is used to change the operating conditions of the process unit due to the change in the value of optimization variables during the optimization process.
Transition optimization was done based on different objective functions taking into account the time of transition phase, invested energy during transition and the amount of off-grade product. Different objective functions results definitely different transition strategies, therefore the choice of right objective function always has to be considered. Large differences can be detected if the optimization task is to decrease the IET as can be seen in Figure 4. If the aim is to minimize the IET, the amount of OGP and the TTP will be higher, which may be not the best choice in the view of financial loss. Applying cost function as objective function in the optimization task can decide which parameter (OGP or IET) is more important in operating point transition. In case of minimizing the TTP and the amount of OGP the optimal transition strategy is similar according to the TTP and the amount of OGP, but there is a slight difference in IET. In case of minimizing the amount of OGP the IET is lower than in case of minimizing the TTP.

Acknowledgement

We would like to express our acknowledgement for the financial support of Széchenyi 2020 under the GINOP-2.2.1-15-2017-00059

References

Chatzidoukas, C., Perkins, J.D., Pistikopoulos, E.N., Kiparissides, C., 2003. Optimal grade transition and selection of closed-loop controllers in a gas-phase olefin polymerization fluidized bed reactor. Chemical Engineering Science, 58, 3643–3658.

Le Digabel, S., 2011. Algorithm 909: NOMAD: Nonlinear Optimization with the MADS Algorithm. ACM Transactions on Mathematical Software, 37, 1–15.

McAuley, K.B., MacGregor, J.F., 1992. Optimal grade transitions in a gas phase polyethylene reactor. AIChE Journal, 38, 1564–1576.

Operator Training Simulator Market Research (2017). Five-year market analysis and technology forecast through 2021. San Francisco, United States. Report ID: GVR5462

Perez, H., Ogunnaike, B., Devasia, S., 2002. Output tracking between operating points for nonlinear processes: Van de Vusse example. IEEE Transactions on Control Systems Technology, 10, 611–617.

Schmidt, R.J., 2005. Industrial catalytic processes—phenol production. Applied Catalysis A: General 280, 89–103.

Sritharan, S., Saharudin, H., 2017. Operator training simulator for ethylene plant. Chemical Engineering Transactions 1621–1626.

Wang X.Q., Vladimir, M., Li Z., Qian F., 2017. Real-time optimization and control of an industrial ethylbenzene dehydrogenation process. Chemical Engineering Transactions, 61, 331–336.