RE-DESIGN OF THE TENNESSEE EASTMAN CHALLENGE PROCESS: AN EIGENVALUE OPTIMIZATION APPROACH

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Abstract

The Tennessee Eastman Challenge Process (TECP) represents an interesting case study within PSE for process control and process optimization purposes. It has been widely addressed by the chemical engineering research community since its publication. The TECP is an open-loop unstable recycle reactor. The eigenvalues of the Jacobean matrix of the system at the base-case steady-state conditions, range from –1968 to +3.07. In absence of feed-back, small perturbations cause large transients reaching shut-down limits within an hour. Operation at open-loop unstable steady-states, even if feasible with feed-back control, is undesirable and should be avoided by proper design. In this contribution, the re-design problem of the TECP is addressed in order to generate an open-loop stable operating condition, by making use of eigenvalue optimization techniques. The objective is to find a new steady state point, such that the whole spectrum of the Jacobean matrix of the system lies in the left half of the complex space. Such a problem corresponds to the design-for-operability discipline, of outstanding importance within the PSE research.

Keywords

Design- for-operability, Eigenvalue optimization, Tenneessee Eastman Process.

Introduction

Operability is a wide and rather subjective concept that may be defined as “the ability of the plant (together with the control strategy) to achieve acceptable static and dynamic operation.” This is a slightly modified version of Wolff’s definition (Wolff et al., 1994). In order to provide a more precise definition of operability, it is usually broken down into a number of properties (elements) of more intuitive meaning, for example stability, flexibility, controllability etc. In particular stability is defined as the condition of the steady state operating points of the plant to be locally asymptotically stable.

Operability is therefore strongly related with the dynamic performance of the process. It is widely accepted that operability features of dynamic systems are determined by design. This suggests the convenience of considering operability features early in the design process and not in later stages where the impact of the modifications is less significant and more expensive.

In fact, design-for-operability has been widely addressed by the chemical engineering research community in the last decades. Several methods have been proposed to tackle such a problem, by making use of linear and non-linear techniques. See Blanco and Bandoni (2003 a) for a review on major approaches for design-for-operability.

The conflicting nature of economic and operability optimization objectives has also arose as a conclusion of such a research.

In particular, several aspects of the design-for-operability problem have been addressed through eigenvalue optimization techniques (Blanco and Bandoni, 2003 a, b). In this contribution, the redesign-for-stability problem will be considered in the context of eigenvalue optimization. The objective is to find a steady-state open-loop operating point of the plant, such that the whole spectrum of the Jacobean matrix of the dynamic system of the process lies in the left half of the complex space.

The rationale behind this is that although feasible operation of open-loop unstable systems is possible by adequate feedback control, such a situation is usually undesirable because of operability and safety reasons and should be avoided by proper design (Luyben et al., 1998).

The proposed strategy will be applied to the study of the TECP, which is an open-loop unstable recycle reactor at its base-case operating point.

Eigenvalue optimization

Local stability of dynamic systems correspond to a Hurwitz condition (Khalil, 1996) on the Jacobean matrix of the process dynamic system $\mathbf{A}(\mathbf{y})(n,n)$, where $\mathbf{y}$ represents the design and/or operating variables. In order to design-for-stability we can formulate the following optimization problem:

$$\begin{aligned} &\min_{\mathbf{y}} \Phi(\mathbf{y}) \\ \text{s.t.}\quad & \mathrm{Re}(\lambda_i(\mathbf{A}(\mathbf{y})) < 0, \quad i = 1,...,n \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ & \mathbf{y} \in \mathrm{Y} = \left\{ \mathbf{y} \middle| \mathbf{y}^l \leq \mathbf{y} \leq \mathbf{y}^u \right\} \end{aligned} \tag{1}$$

In general, $\Phi(\mathbf{y})$ is an economic objective function, $\mathbf{h}(\mathbf{y})$ is the set of equality constraints (mass and energy steady-state balances, geometric and equilibrium relationships, etc.), $\mathbf{g}(\mathbf{y})$ is the set of inequalities (operational and design constraints), and λ_i are the eigenvalues. Several approaches have been proposed to handle the difficult aspects of problem (1), mainly the impossibility of obtaining explicit expressions for eigenvalues of even small size matrices and the non-differentiability of such expressions if available. A "classic" reformulation of (1) in terms of Lyapunov's matrix identity is (2) (see Blanco and Bandoni (2003 b) for details). Here, $\mathbf{P}$ is a symmetric matrix, defined by Lyapunov's equation, whose positive definiteness is established by ensuring the determinants of its inverse principal minors, $\mathbf{P}_i^{-1}$, are strictly positive.

Problem (2) is a standard NLP problem, since the determinants are themselves smooth, and can therefore be solved with standard gradient based algorithms. Determinants may be efficiently evaluated from $\mathbf{y}$ for provision to the solver.

$$\begin{aligned} &\min_{\mathbf{y}} \Phi(\mathbf{y}) \\ \text{s.t.}\quad & \mathbf{A}^T(\mathbf{y})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}) + \mathbf{I} = \mathbf{0} \\ & \det(\mathbf{P}_i^{-1}) \geq \xi \quad i = 1,...,n \\ & \xi > 0 \\ & \mathbf{h}(\mathbf{y}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}) \leq \mathbf{0} \\ & \mathbf{y} \in \mathrm{Y} \end{aligned} \tag{2}$$

The procedure is as follows: (i) given $\mathbf{y}$, the Jacobean matrix $\mathbf{A}(\mathbf{y})$ can be calculated either numerically or analytically, (ii) then the Lyapunov equation is solved for $\mathbf{P}$, which is inverted to obtain matrix $\mathbf{P}^{-1}$, (iii) finally the determinants of the principal minors of matrix $\mathbf{P}^{-1}$, $\det(\mathbf{P}_i^{-1})$ are evaluated. A feasible starting point is required for the optimization. Details on the above algorithm can be found in Blanco (2003).

TECP

The TECP has been introduced to the PSE research community in Downs and Vogel (1993). Since its publication it has received considerable attention in the fields of plant-wide control and optimization. The TECP consists of a reactor/separator/recycle arrangement involving two principal simultaneous gas-liquid exothermic reactions, and two by product additional reactions. Unit operations include a reactor, a partial condenser, a recycle compressor and a stripper. The flowsheet for this process is shown in Figure 1. The reader is referred to Downs and Vogel (1993) for the detailed description of the process.

The TECP have motivated the development of several mechanistic models to address its steady-state and dynamic study.

In particular Ricker and Lee (1995 a) developed a mechanistic/parametric-adjustable dynamic model in order to reproduce the essential process characteristics without introducing unnecessary detail. Major simplifications of such a model include the elimination of energy balances by considering reactor and separator temperatures as manipulated variables, the elimination of the compressor model by considering its corresponding flow as a manipulation as well and the avoidance of a detailed modeling of the stripper. The resulting model has 26 states (mass balances in the different sectors of the process) and 10 manipulations (degrees of freedom), which comprise main flow rates and reactor and separator temperatures.

Further refinements for the model were introduced later in Jockenhoevel et al. (2003) where energy balances for the different units are effectively considered.

The TECP is an open-loop unstable plant, which reaches shut down limits within about an hour in absence of feedback control, even for modest disturbances. This is shown by simulation in Downs and Vogel (1993) and also demonstrated by a linear eigenvalue analysis in Ricker and Lee (1995 b) where a range of eigenvalues of the process system Jacobean matrix from -1968 to 3.07 is reported.

The model proposed in Ricker and Lee (1995 a) as well the one in Jockenhoevel et al. (2003) reproduce such open-loop unstable behavior.

In fact most studies on plant-wide control on the TECP assume a previous stabilization of the plant by means of PI controllers (Ricker and Lee, 1995 b; Jockenhoevel et al., 2003).

It is the purpose of this work to apply the eigenvalue optimization strategy proposed in the previous section to find a new operating point of TECP such that verify asymptotic stability, which is a Hurwitz condition on the dynamic system Jacobean matrix.

Eigenvalue optimization of the TECP

The NLP problem described by Eqn. 2 was formulated for the TECP model proposed in Ricker and Lee (1995 a). The reader is referred to that article for a detailed description of modeling assumptions, system equations, system data and nomenclature.

Previous studies on steady state optimal operation of the TECP were performed in Ricker (1995). In particular a minimum cost problem was solved for the base-case proposed by Downs and Vogel (1993) showing that significant improvements were possible.

The total cost objective function (OF) proposed by Downs and Vogel (1993) considers a term by lost of product and raw material in the purge stream (stream F9), a term by lost of raw material in the product stream (stream F11) a term by compression work (related to recycle stream F8) and a term by heating.

During our steady state simulation experiences, it was noticed that an increase of about seven times in the recycle flow-rate (stream F8) had a stabilizing effect, producing the whole spectrum of the Jacobean matrix of the system to lie in the left half of the complex plane.

Since this variable (F8) had a strong effect on the cost objective function due to compression work (Wc), a simple expression for an isentropic compressor (not considered in Ricker and Lee model) which relates pressure increase and flow-rate (Smith and Van Ness, 1989) was applied to model such a term.

The heating cost term was neglected since energy balances are not included in the considered model.

In order to demonstrate this approach and also to consider the cost of open loop stability we consider the following cases:

TECP 1: The minimum cost function was minimized subject to the steady state model of the process using the base-case data as the starting point for the optimization.

TECP 2: The minimum cost function was minimized subject to the steady state model of the process plus additional constraints in order to ensure Hurwitz stability (Problem (2)). The starting point for the optimization ($\mathbf{y}^0$) corresponds to a feasible steady state regarding stability ($\mathrm{Re}\{\lambda_i[A(\mathbf{y}^0)]\}<0$). All the nonlinear programming problems were solved with a successive quadratic programming algorithm (Biegler and Cuthrell, 1985). Results for cases TECP1 and TECP2 are reported in Table 1. Only the most relevant variables are presented.

Table 1: Cases TECP1 and TECP2

Variable	units	TECP1	TECP2
F1	kmol/h	6.892	9.999E-006
F2	kmol/h	100.000	55.649
F3	kmol/h	75.000	9.481
F4	kmol/h	346.149	130.786
F8	kmol/h	1000.000	6790.000
F9	kmol/h	6.994	1.261
F10	kmol/h	219.521	69.593
F11	kmol/h	176.089	64.522
Tr	K	388.163	395.016
Ts	K	334.945	360.764
Ps	kPa	2855.507	1304.782
Pr	kPa	2895.000	2895.000
Pm	kPa	3116.896	11831.668
Wc	kW	68.308	15165.700
OF	$/h	42.260	824.210

The real parts of the eigenvalues for case TECP1 range from -2416.84 to 0.21, while those corresponding to case TECP2 range from -1785.35 to -3.19E-9.

Case TECP1, which is close to Downs and Vogel (1993) base-case, is open loop unstable while TECP2 is a Hurwitz stable (almost marginally) plant as expected.

The operating points corresponding to both cases are notoriously different. This is mainly reflected in the recycle flow-rate stream, which is about seven times the value of TECP1 in TECP2, and in the working pressure (Pm) of the mixing zone of the process (where the recycle stream is mixed with the feed streams), which is about four times the value of TECP1 in TECP2. These variables have a strong effect in the compressor work (Wc), which increases linearly with F8, and in a nonlinear fashion with Pm. This effect translates to the objective function, which is about twenty times higher for TECP2.

These are in fact expected results considering the conflicting tradeoff between economic and operability objectives. A desirable operating condition was achieved, open-loop stability, but at the expense of a notable increase in operating costs. It should be noted that the new operating condition might be hard to implement due to the very high pressure in the mixing zone.

It is also remarkable that the feed streams (F1, F2, F3 and F4) as well as the outlet streams (F9 and F11) are greatly reduced in TECP2 regarding TECP1. This implies that products are being produced at a much lower rate and that a larger amount of raw material is being recycled in the system in TECP2.

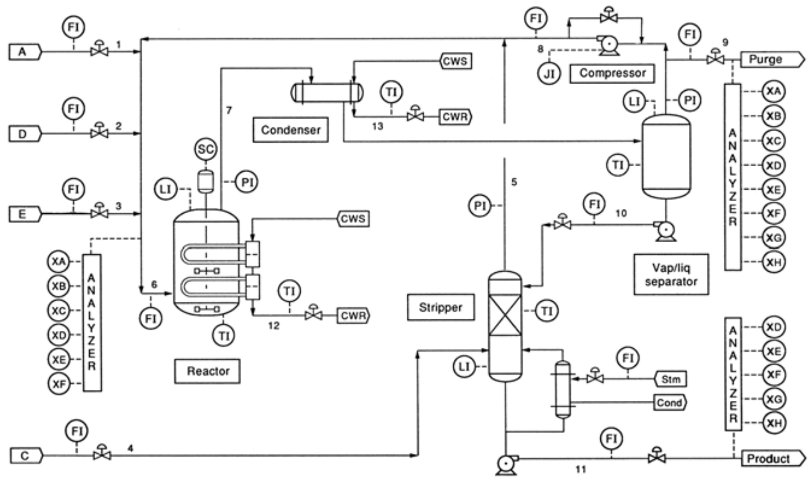

Figure 1: Tennessee Eastman Process Flowsheet

Conclusions

In this contribution an eigenvalue optimization based design-for-operability study was performed on the TECP.

The TECP (base-case) presents open-loop instability in absence of feedback control, a particularly challenging feature for dynamic operation and plant-wide control of processes.

The main purpose of the present study was to find a new steady state operating point of the process, such that the system verifies open-loop dynamic asymptotic stability, a desirable feature from an operating point of view.

The new operating condition, as result of solving Problem (2), leads to Hurwitz stability at the expense of a much higher total operating cost, mainly due to a larger required compression work in the recycle stream.

Such a result is expected indeed since economics and operability (stability for example) are known to have a conflicting nature from an optimization standpoint.

Future work will consider more sophisticated models of the TECP (Jockenhoevel et al., 2003) and the possibility of modifying design variables such as equipment sizes.

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