

# Interaction between process design and process operability of chemical processes: an eigenvalue optimization approach

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Received 6 February 2003; accepted 7 February 2003

## Abstract

An increasing effort is being devoted to consider controllability issues (or in a wider sense operability issues) at the process design stage. Controllability has mainly to do with dynamics in the face of disturbances. One philosophy for the integration of design and controllability is to explicitly consider dynamic elements within the process design formulation. An outstanding feature of dynamics is stability, which is related with the spectrum (set of eigenvalues) of the dynamic system Jacobian matrix. Dynamic convergence speed may also be analyzed in terms of the eigenvalues of the matrix from a Lyapunov function related to the Jacobian of the system. It is the purpose of this contribution to formulate and solve the chemical process design problem, considering process dynamics from an eigenvalue optimization approach.

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*Keywords:* Process operability; Process dynamics; Eigenvalue optimization

## 1. Introduction

The underlying idea behind the interaction between process design and process operability is to perform some sort of operability assessment at the early stages of the process design procedure in order to generate a design with good operability characteristics. Such an interaction becomes necessary since the traditional approach to process design, just interested in steady-state economic optimality, or little more, could lead to difficult or even impossible to operate processes.

Process operability is a wide concept, which is made up by an amount of elements. As pointed out by Wolff, Perkins and Skogestad (1994), outstanding elements of operability are optimality, stability, flexibility and controllability. Risk and environmental issues are also becoming increasingly important within the operability definition.

Optimality in an economical sense is a natural goal of chemical process design. Open-loop local asymptotic

stability of the operating point, which implies the existence of a certain domain of attraction for such equilibrium, is a major feature and can by itself decide the fate of the operation. Then, although operation at an open-loop unstable steady-state may be feasible under feedback control, it is undesirable and should be avoided by proper design. Flexibility implies ensuring feasible regions of steady state operation in the face of disturbances and parametric uncertainty. Controllability has to do with closed-loop dynamic response quality between different steady states, as a result of disturbance-rejection and servo-actions (the latter case is also referred as switchability). A high quality transient response involves a fast and not very oscillating trajectory, without violation of potential path constraints.

There exists an increasing interest in integrating these and other operability elements at the design stage since it is known that operability strongly depends on design. In the last couple of decades an increasing effort has been devoted to the development of operability analysis tools. In terms of philosophies we can mention three major approaches to the design-for-operability problem: heuristic approach, operability measures and complete

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integration. See Lewin (1999) for a comprehensive review on the subject.

Design heuristics approach relies on well proved recipes based mostly on experience. Within such an approach the book by Douglas (1988) on conceptual design is remarkable. It makes wide use of experience based knowledge in the form of rules of thumb.

Operability measures describe particular operability features and become valuable tools in order to screen or classify alternative designs regarding a particular operability issue (Barton, Chan & Perkins, 1991). A particularly important set of operability measures is that of open-loop controllability and resiliency indices. Such indices are mostly based on linearized models. We can mention Relative Gain Array and singular value decomposition techniques among others.

Integration between process design and process operability implies the explicit inclusion of operability elements within the process design formulation, in order to generate inherently operable designs. A number of alternative formulations of the design-for-operability integration approach have been proposed. For example, Luyben and Floudas (1994) proposed a multi-objective optimization approach between economic and operability (typically a controllability or resiliency index) objectives. Another ambitious formulation within this category is that of Mohideen, Perkins and Pistikopoulos (1996) in which a mixed-integer non-linear programming problem is posed, such that both, a design superstructure and a Proportional-Integral feedback control superstructure are simultaneously solved.

All the previous approaches require some extent of non-linear dynamic simulation to validate the resulting design. This used to be a time consuming and computationally demanding activity. Current practice in the design-for-operability problem involves some degree of combination of all of the three approaches. However, the trend is in the sense of complete integration, although the complexity in modeling and solving the problem increases towards integration.

In this contribution, which is intended to fit in the last category, an integrating approach is proposed to consider dynamics within the process design optimization problem making use of the direct relation between system dynamics and eigenvalue theory. Dynamic stability has to do with the set of eigenvalues of the dynamic system Jacobian matrix ( $A$ ). Transient response speed has also to do with the spectrum of the matrix from the Lyapunov identity related to  $A$ .

Lyapunov's theory has been applied some decades ago to the study of dynamic stability of chemical processes (Berger & Perlmutter, 1964, for example) but mainly from an analysis point of view. Energy function methods have been almost neglected from since in chemical engineering literature. This responds to inherent drawbacks in the application of such techniques to

the difficult non-linear dynamics of chemical processes. It is our belief, however, that energy function techniques are still valuable in chemical process dynamics and this contribution intends to be a step in such direction.

Eigenvalue optimization is a subject of interest in many fields of applied science (Lewis & Overton, 1996) and present challenging algorithmic features since models that involve eigenvalues (as objective function and/or constraints) may become non-smooth when coalescing eigenvalues appear (Ringertz, 1997).

Two different formulations are proposed in this contribution: design for local asymptotically stable operating points and design for fast local transients. The former is applied to the economically optimal design problem and the later to the optimal controller-tuning problem.

The proposed methodology is known to overcome several drawbacks that arise when eigenvalues are present in optimization models: the lack of analytic expressions for the eigenvalues of larger than 4 by 4 matrices and the potential non-smoothness of the resulting formulations as already commented. It is also expected to be a step in the sense of avoiding the tedious dynamic simulation at the process design stage.

In the following sections, most relevant theoretical topics concerning this contribution are briefly introduced, then proposed formulations are presented and outlined through a simple motivating example and finally applied to the design and control of simple, although meaningful, chemical engineering models.

## 2. Lyapunov's stability theory

For a general non-linear dynamic system  $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ , local analysis of the steady-state equilibrium  $\mathbf{x}_{ss}$  is the best we can do regarding stability. For asymptotic local dynamic stability we understand the existence of a certain neighborhood around the equilibrium point within which asymptotically stable trajectories originate. This means that any trajectory starting inside this neighborhood also called stability region or domain of attraction (Fig. 1), approaches the equilibrium point as

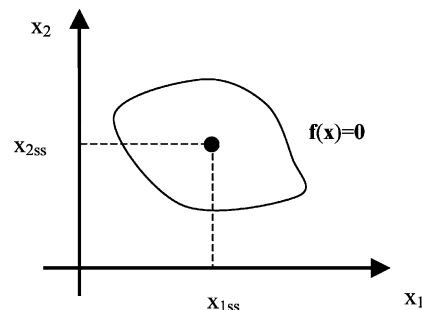


Fig. 1. Domain of attraction for a two states system.

time increases. At the moment we are not interested in the shape or size of such a region but just on its existence. In the present section, some basic ideas from dynamic systems theory are reviewed. See, for example, Vidyasagar (1993) for a complete analysis.

### 2.1. Lyapunov's linearization method

Consider the free, autonomous (time invariant) dynamic system:

$$\frac{dx}{dt} = f(x), \quad f(0) = 0 \quad (1)$$

where  $x$ , represents the deviation state vector. We can put  $f(x) = Ax + f_1(x)$ , where  $A = [\partial f / \partial x]_{x=0}$ . Then, it can be proved (Vidyasagar, 1993) that  $0$  is an exponentially stable local equilibrium of Eq. (1) if all eigenvalues of  $A$  have negative real parts (if  $A$  is a Hurwitz matrix). Lyapunov's stability theory provides an energetic approach to stability. Quadratic form  $V(x) = x^T P x$  is a suitable Lyapunov function for system (Eq. (1)) (which means that matrix  $A$  is a Hurwitz matrix) if matrix  $P$  is positive definite (real and symmetric) and the energy function derivative with respect to time  $\dot{V}(x) = -x^T Q x + 2x^T P f_1(x)$ , verifies that matrix  $Q$  is also positive definite (real and symmetric). Matrices  $A$ ,  $P$  and  $Q$  are related through Lyapunov's matrix equality:

$$A^T P + P A + Q = 0. \quad (2)$$

Usual practice is to choose matrix  $Q$  to be a positive definite symmetric matrix (in general the identity matrix). Therefore, provided  $A$ , Eq. (2) can be solved for  $P$ , also symmetric. If  $P$  is positive definite, then  $A$  is a Hurwitz matrix. Furthermore (Vidyasagar, 1993), define  $B_r = \{x \in \mathbb{R}^n \mid \|x\| < r\}$  such that (let  $\lambda_i$  denote eigenvalue):

$$\frac{\|f_1(x)\|}{\|x\|} < \frac{\lambda_{\min}(Q)}{2\lambda_{\max}(P)}, \quad \forall x \in B_r. \quad (3)$$

It stands that  $\dot{V}(x) < 0$ , whenever  $x \in B_r$  and  $x \neq 0$ . Therefore,  $B_r$ , provides an estimate of the domain of attraction of  $0$ , that is, the region of the state space where asymptotically stable trajectories are generated.

### 2.2. Estimation of transients

Consider now parameter  $\eta$ , defined as:  $\eta = \min_x \{(-dV(x)/dt)/V(x)\}$ , which may be loosely regarded as the reciprocal of the largest time constant descriptive of the motion over the region of asymptotic stability and is, therefore, a figure of merit for the control system. A large value of  $\eta$  indicates that the system returns rapidly to the origin. In particular, from Eq. (2), it is found (Koppel, 1968) that

$$\eta = \lambda_{\min}(P^{-1}Q) \quad (4)$$

## 3. Eigenvalue optimization

Eigenvalues of matrices play important roles in many fields of applied mathematics to engineering. For certain applications it might be desirable to formulate optimization problems involving eigenvalues of matrices as objective functions and/or constraints.

Our particular interest in eigenvalue optimization is related to the contents of the previous section where the connections between eigenvalues and system dynamics (mostly the stability issue) were roughly established.

It is the purpose of this section to provide a brief overview of the most relevant topics on eigenvalue optimization. For a comprehensive survey on the subject, which also includes an historical account of the development of the field, see Lewis and Overton (1996).

The main difficulty arising in eigenvalue optimization problems is the potential coalescence of eigenvalues. The eigenvalues of a matrix with differentiable elements (smooth in the optimization variables) are themselves non-differentiable (non-smooth) at the points where coalescence occurs. It is also frequent that the optimization objective tends to make the eigenvalues coalesce at the solutions (Overton, 1992). The following classic example illustrates this point. Consider the following matrix:

$$A(x) = \begin{bmatrix} 1 + x_1 & x_2 \\ x_2 & 1 - x_1 \end{bmatrix}$$

whose eigenvalues are:

$$1 \pm \sqrt{x_1^2 + x_2^2}$$

It can be seen that the maximum eigenvalue is minimized by  $x_1 = x_2 = 0$ . Clearly the maximum eigenvalue is not a smooth function in such a point. Then it is necessary to develop specialized optimization methods to overcome this difficulty.

Besides this potential non-smoothness, there exist the impossibility of obtaining mathematical expressions for the eigenvalues of larger than 4 by 4 systems (Kokossis & Floudas, 1994). This makes it impossible to include eigenvalues within the optimization model in a straightforward manner (as objectives and/or constraints). Furthermore, even in the cases where analytical expressions can be obtained, their usual high complexity and non-convexity make difficult to standard NLP solvers to cope with them.

An amount of well-developed theory is available for the case of eigenvalue optimization of symmetric

matrices depending linearly on the optimization variables and subject to linear constraints. The general non-linear unsymmetric case has been far less boarded although some meaningful results have been obtained in the field of structural design (Ringertz, 1997).

This contribution is an attempt to apply some of those results in the chemical engineering area. Just an introduction to the main ideas is going to be presented in the remainder of this section since details are provided in the following sections where specific problems are proposed and analyzed through examples.

Most of the eigenvalue optimization theory has been developed for real symmetric matrices. It is known that such matrices have real eigenvalues. Unsymmetric matrices, on the other hand, have complex eigenvalues in general. It is possible, however, to translate the constraint on the real part of the eigenvalues of a real unsymmetric matrix (say  $\mathbf{A}$ ) to be negative, into a positive definiteness condition on a real symmetric matrix ( $\mathbf{P}$ ) through Lyapunov's matrix equality Eq. (2). Since it is a sufficient and necessary condition for a real symmetric matrix to be positive definite its eigenvalues to be positive, the condition on the eigenvalues of the 'difficult' unsymmetric matrix  $\mathbf{A}$  is translated into another condition on the eigenvalues of the 'not-so-difficult' symmetric matrix  $\mathbf{P}$ .

In order to avoid the potential non-smoothness arising in eigenvalue optimization as already commented, interior-point/logarithmic-barrier-transformation techniques have been successfully applied (Ringertz, 1997). For a comprehensive reference of interior-point optimization, see Fiacco and McCormick (1990). The underlying idea behind interior-point minimization, in particular that which makes use of logarithmic penalty functions, is to reduce in value the objective function, simultaneously assuring non-violation of the constraints. The strategy consists in penalizing the objective function with logarithmic terms whose arguments are the constraints themselves expressed in the form of greater than zero.

Making use of logarithmic and matrix determinant properties, it will be shown that the  $n$  (potentially non-smooth) constraints on the eigenvalues of matrix  $\mathbf{P}$  (where  $n$  is the size of the dynamic system) may be comprised into one simple logarithmic term involving the determinant of matrix  $\mathbf{P}$  which is a smooth function of the optimization variables.

#### 4. Optimal design of stable processes

The basic general problem of (steady-state) chemical process design may be posed as a constrained, non-linear programming problem under uncertainty. Local stability at the steady-state equilibrium point requires the jacobian (unsymmetric) matrix of the dynamic

system ( $\mathbf{A}$ ) to be Hurwitz. In terms of eigenvalues, the design problem may be formulated as:

$$\begin{aligned} & \min_{\mathbf{y}} \Phi(\mathbf{y}, \boldsymbol{\theta}) \\ \text{s.t. } & \operatorname{Re}(\lambda_i(\mathbf{A}(\mathbf{y}, \boldsymbol{\theta}))) < 0, \quad i = 1, \dots, n \\ & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in Y, \quad \boldsymbol{\theta} \in \Omega \end{aligned} \quad (5)$$

where,  $\mathbf{y}$  is the vector of optimization variables and  $\mathbf{u}$  the vector of uncertainty. In general,  $\Phi(\mathbf{y}, \mathbf{u})$  is an economic type objective function,  $\mathbf{h}(\mathbf{y}, \mathbf{u})$  is the set of equality constraints (mass and energy steady-state balances, geometric and equilibria relationships, etc.) and  $\mathbf{g}(\mathbf{y}, \mathbf{u})$  is the set of inequalities (operational and design constraints).

Such a problem has been addressed by Kokossis and Floudas (1994) and applied to the meaningful problem of complex reactor network synthesis. In their work the authors propose a matrix measure relaxation approach for bounding the eigenvalues of  $\mathbf{A}$  in order to ensure local dynamic asymptotic stability of the design. With a similar philosophy, dynamics is explicitly considered within the design problem from an eigenvalue optimization approach in this contribution.

Such a problem may be non-smooth because of the eigenvalue constraints (Ringertz, 1997). In order to avoid the difficulties of solving problem Eq. (5), the stability issue is considered by adding Lyapunov's Eq. (2) to the steady state model of the system and requiring positive definiteness on symmetric matrix  $\mathbf{P} = [p_{ij}]$  ( $\mathbf{P} > \mathbf{0}$ ) provided that matrix  $\mathbf{Q}$  is symmetric and positive definite (usually  $\mathbf{Q} = \mathbf{I}$ ):

$$\begin{aligned} & \min_{\mathbf{y}} \Phi(\mathbf{y}, \boldsymbol{\theta}) \\ \text{s.t. } & \mathbf{A}^T(\mathbf{y}, \boldsymbol{\theta})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}, \boldsymbol{\theta}) + \mathbf{I} = \mathbf{0} \\ & \mathbf{P} > \mathbf{0} \\ & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in Y, \quad \boldsymbol{\theta} \in \Omega \end{aligned} \quad (6)$$

The above is a non-linear semi-definite programming problem because of the positive definiteness requirement on matrix  $\mathbf{P}$ , which implies that  $\lambda_i(\mathbf{P}) > 0$ ,  $i = 1, \dots, n$ . Since Lyapunov's equation might force matrix  $\mathbf{P}$  to become unbounded when the largest eigenvalue of  $\mathbf{A}$  approaches zero, an equivalent, but numerically better posed constraint is  $\mathbf{P}^{-1} > \mathbf{0}$ , which implies  $\lambda_i(\mathbf{P}^{-1}) > 0$ ,  $i = 1, \dots, n$ :

$$\begin{aligned} & \min_{\mathbf{y}} \Phi(\mathbf{y}, \boldsymbol{\theta}) \\ \text{s.t. } & \mathbf{A}^T(\mathbf{y}, \boldsymbol{\theta})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}, \boldsymbol{\theta}) + \mathbf{I} = \mathbf{0} \\ & \lambda_i(\mathbf{P}^{-1}) > 0, \quad i = 1, \dots, n \\ & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in Y, \quad \boldsymbol{\theta} \in \Omega \end{aligned} \quad (7)$$

Such a problem may be efficiently tackled via interior-



point methods. In terms of a logarithmic barrier transformation, problem Eq. (7) can be reformulated as (Ringertz, 1997):

$$\begin{aligned} & \min_{\mathbf{y}} \{ \Phi(\mathbf{y}, \boldsymbol{\theta}) + \mu \log(\det \mathbf{P}) \} \\ \text{s.t. } & \mathbf{A}^T(\mathbf{y}, \boldsymbol{\theta})\mathbf{P} + \mathbf{P}\mathbf{A}(\mathbf{y}, \boldsymbol{\theta}) + \mathbf{I} = \mathbf{0} \\ & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in \mathbf{Y}, \boldsymbol{\theta} \in \Omega \end{aligned} \quad (8)$$

since  $\sum_{i=1}^n \log(\lambda_i(\mathbf{P}^{-1})) = \log \prod_{i=1}^n \lambda_i(\mathbf{P}^{-1}) = \log(\det(\mathbf{P}^{-1})) = -\log(\det(\mathbf{P}))$ . From a feasible starting-point ( $\mathbf{P} \succ 0$ ), the solution of Eq. (8) converges to the solution of Eq. (7) for a decreasing sequence of barrier parameters  $\{\mu^k\}$  as  $\mu^k \rightarrow 0$ . Positive definiteness on matrix  $\mathbf{P}$  should be ensured at the solution since  $\det(\mathbf{P}) > 0$  is not a sufficient condition.

#### 4.1. Algorithmic insight

Before going on further, some comments on algorithmic issues should be done. The above described interior-point/logarithmic-barrier-transformation problems are solved in the present contribution with standard NLP solvers and positive definiteness of matrix  $\mathbf{P}$  checked at the solution since, as already commented, determinant of matrix  $\mathbf{P}$  being positive is not a sufficient condition for matrix  $\mathbf{P}$  being positive definite.

Such an approach has several drawbacks. In interior-point/logarithmic-barrier-transformation techniques, the constraints (expressed as greater than zero) are arguments of logarithmic functions. Along the optimization process, it may happen that some constraint become zero or negative undetermining the logarithm and producing a runtime error. In order to cope with such situations interior-point/logarithmic-barrier-transformation optimization algorithms use to check constraint feasibility before evaluating the objective function, and if violation verifies, backtracking is performed on the line-search until feasibility is achieved (bear in mind that feasibility in the starting point is required in interior point techniques).

In our particular optimization problem, matrix  $\mathbf{P}$  positive definiteness checking convenience is two-fold. It may happen that along the optimization an odd number of eigenvalues change sign simultaneously making matrix  $\mathbf{P}$  determinant negative and runtime error occurrence. Even worse, it may happen that an even number of eigenvalues change sign simultaneously such that matrix  $\mathbf{P}$  determinant remains positive but loosing positive definiteness condition on  $\mathbf{P}$  and hence local stability.

For the general case, an algorithm that checks positive definiteness on  $\mathbf{P}$  in each iterate (by checking its eigenvalues, for example) and the step-length parameter in line-search reduced until positive definiteness

condition is achieved should be applied (Fig. 2). Such an algorithm has been applied in the solution of large-scale models within the structural design field (Ringertz, 1997).

#### 4.2. Parametric uncertainty

Formulation Eq. (8) involves uncertain parameters and represents, therefore, an infinite dimensional optimization problem. An amount of approaches has been presented for optimal process design under uncertainty within deterministic, probabilistic and flexibility-analysis philosophies (Pistikopoulos & Ierapetritou, 1995).

In this work a classic deterministic-based approximation is considered, which drives to a multi-period program when disturbance and parametric uncertainty vectors are specified in advance according to a certain realization. A general formulation of the problem may be:

$$\begin{aligned} & \min_{\mathbf{y}} \mathbf{P}(\mathbf{y}, \boldsymbol{\theta}) \\ \text{s.t. } & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in \mathbf{Y} = \{ \mathbf{y} | \mathbf{y}^l \leq \mathbf{y} \leq \mathbf{y}^u \} \\ & \boldsymbol{\theta} \in \Omega = \{ \boldsymbol{\theta} | \boldsymbol{\theta}^l \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^u \} \end{aligned} \quad (9)$$

where  $\mathbf{y}$  is the vector of optimization variables and  $\mathbf{u}$  the vector of uncertainty. Vector  $\mathbf{y}$  comprises design, control and state optimization variables, with usual definitions each. The underlying idea of the deterministic-based approach for design under uncertainty is to transform the original, semi-infinite in  $\mathbf{u}$ , optimization problem into a deterministic approximation by specifying in advance a number of uncertain parameter realizations, giving rise to the following multi-period program:

$$\begin{aligned} & \min_{\mathbf{y}} \sum_{i=1}^N \mathbf{P}(\mathbf{y}^i, \boldsymbol{\theta}^i) \\ \text{s.t. } & \left. \begin{aligned} & \mathbf{h}^i(\mathbf{y}^i, \boldsymbol{\theta}^i) = \mathbf{0} \\ & \mathbf{g}^i(\mathbf{y}^i, \boldsymbol{\theta}^i) \leq \mathbf{0} \end{aligned} \right\} \quad i = 1, \dots, N \\ & \mathbf{y}^i \in \mathbf{Y}, \boldsymbol{\theta}^i \in \Omega \end{aligned} \quad (10)$$

Note that a subset of variables of vector  $\mathbf{y}^i$ , the so-called design variables, remains the same for all the periods since it corresponds to the vector of degrees of freedom of the algebraic equation system of the model.

It should be emphasized that problem Eq. (10) is an approximation to the direct solution of problem Eq. (9) due to its discrete nature. Such an approach has been adopted here to cope with uncertainty because of its straightforward application.

The related multi-period formulation Eq. (10), of Eq. (8) is:

$$\min_{\mathbf{y}^i} \left\{ \sum_{i=1}^N \Phi(\mathbf{y}^i, \boldsymbol{\theta}^i) + \mu \sum_{i=1}^N \log(\det \mathbf{P}^i) \right\}$$

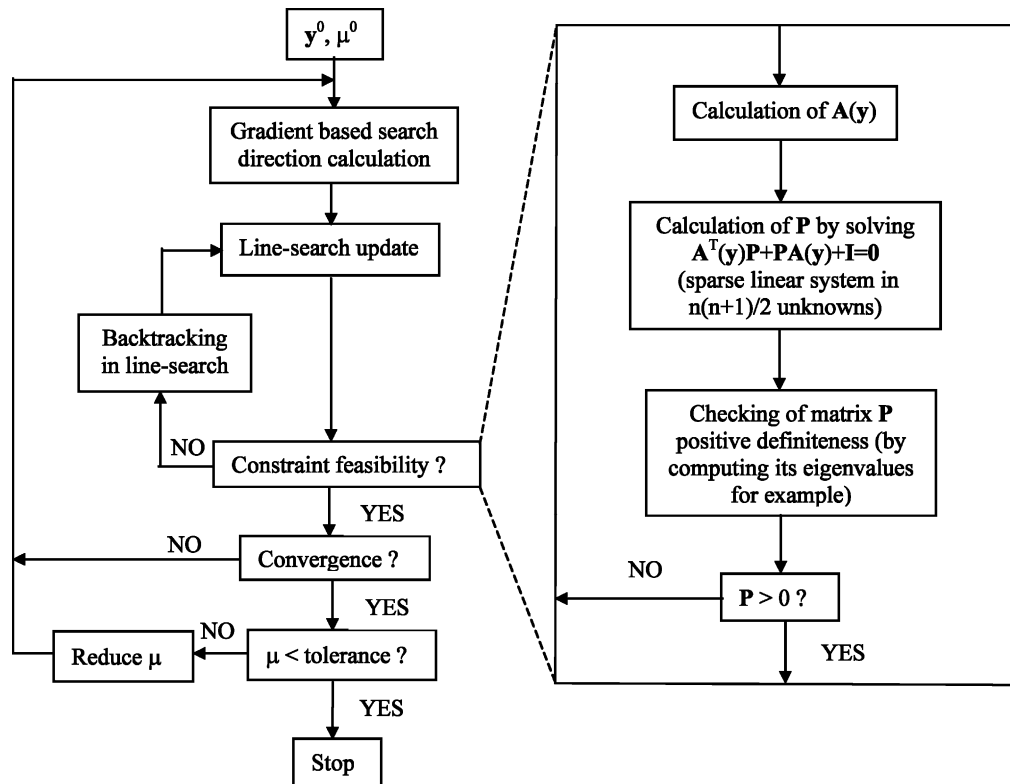


Fig. 2. Suggested algorithm for large-scale models.

$$\begin{aligned}
 \text{s.t. } & \left. \begin{aligned} & \mathbf{A}^T(\mathbf{y}^i, \boldsymbol{\theta}^i)\mathbf{P}^i + \mathbf{P}^i\mathbf{A}(\mathbf{y}^i, \boldsymbol{\theta}^i) + \mathbf{I} = \mathbf{0} \\ & \mathbf{h}^i(\mathbf{y}^i, \boldsymbol{\theta}^i) = \mathbf{0} \\ & \mathbf{g}^i(\mathbf{y}^i, \boldsymbol{\theta}^i) \leq \mathbf{0} \end{aligned} \right\} i = 1, \dots, N \\
 & \mathbf{y}^i \in \mathbf{Y}, \boldsymbol{\theta}^i \in \Omega
 \end{aligned} \quad (11)$$

By means of the above formulation the existence of a certain domain of attraction for every point of the uncertain parameter vector realization can be ensured. This is roughly sketched in Fig. 3 for a two states system and two points of uncertainty realization.

As already commented, constraint feasibility (which implies local stability) is only ensured at the provided discrete realization and not in the whole parameter space. Other strategies to cope with uncertainty in a more elegant and conclusive fashion could be applied (Raspanti, Bandoni & Biegler, 2000).

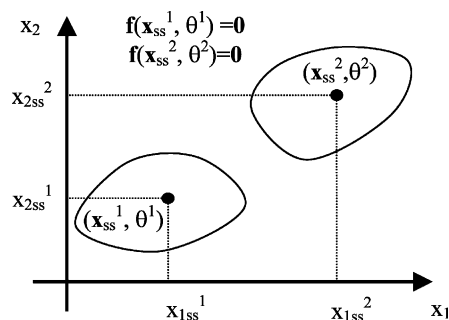


Fig. 3. Local stability for uncertainty realization.

The above ideas are illustrated through the following simple extended example from Kokossis and Floudas (1994).

#### 4.3. Motivating example

Consider the optimization problem:

$$\min x_2^2$$

associated with the dynamical system:

$$\dot{x}_1 = x_1^2 + x_2^2 - c$$

$$\dot{x}_2 = x_1^2 + x_2 - 4p$$

and variable restrictions:

$$0 \leq p \leq 1$$

$$x_1 \leq 0$$

$$x_2 \geq 0$$

$x_1$  and  $x_2$  are the state variables,  $p$  is a design parameter and  $c$  is an uncertain parameter expected to vary in the range  $\{0.9, 1.05\}$ .

It is interesting to note that for certain uncertain parameter realizations ( $c = 1$ , for example) the corresponding steady state optimization problem of the above model (with no stability constraints) drives to an unstable solution as reported in Kokossis and Floudas (1994), although a better optimum is obtained.

The system jacobian matrix of the dynamic system is  $\mathbf{A} = [a_{ij}]$ :

$$\mathbf{A} = \begin{bmatrix} 2x_1 & 2x_2 \\ 2x_1 & 1 \end{bmatrix}$$

In order to consider the stability issue, the model is formulated as Eq. (8):

$$\min\{x_2^2 + \mu \log(\det \mathbf{P})\}$$

s.t. Jacobian matrix elements definition

$$a_{11} = 2x_1$$

$$a_{12} = 2x_2$$

$$a_{21} = 2x_1$$

$$a_{22} = 1$$

Lyapunov's equation elements

$$0 = 2a_{11}p_{11} + 2a_{21}p_{12} + 1$$

$$0 = a_{11}p_{12} + a_{21}p_{22} + a_{12}p_{11} + a_{22}p_{12}$$

$$0 = 2a_{12}p_{12} + 2a_{22}p_{22} + 1$$

Determinant definition

$$\det \mathbf{P} = p_{11}p_{22} - p_{12}^2$$

Steady state equations

$$0 = x_1^2 + x_2^2 - c$$

$$0 = x_1^2 + x_2 - 4p$$

Variable constraints

$$0 \leq p \leq 1$$

$$x_1 \leq 0$$

$$x_2 \geq 0$$

Parameter  $c$  realization is assumed to be  $\{0.90, 0.95, 1.00, 1.05\}$ , and the above model posed as Eq. (11). Table 1 summarizes the optimization results.

The problem was solved with GAMS/CONOPT2 (Brooke, Kendrick & Meeraus, 1996). As expected, corresponding Jacobian matrices are Hurwitz and then local stability is verified for the proposed parameter realization.

As can be concluded by inspection of the resulting spectra, the system verifies different local convergence behavior for the different parameter realization points,

from fast non-oscillating response ( $c = 0.95$ ) to slow oscillating transients ( $c = 1.05$ ).

It is also noticeable that almost critical stability ( $\text{Re}(\lambda_i) \cong 0$ ) is achieved for  $c = 0.95$  and  $1.05$ . Critical stability is dangerous in the face of parametric uncertainty since small perturbations may force the eigenvalues of the system to become unstable. Therefore, certain stability margin might be desirable. As already commented the proposed multi-period approach to cope with uncertainty is not conclusive since local stability is only ensured at the considered discrete values and not for the whole uncertain space. A more general approach to flexibility (Raspanti et al., 2000) in order to ensure robust stability will be considered for future research.

The eigenstructure of  $\mathbf{A}$  is related to the value of the determinants of the leading minors of  $\mathbf{P}$  in a non-evident way. The final values of such determinants depend on how small barrier parameter  $\mu$  is allowed to become. It was observed that the smaller the  $\mu$ , the closest the system to critical stability. This suggests the conflicting nature between the 'cost objective' and the 'stability objective'. Parameter  $\mu$  final value might be a way to establish the desirable stability margins. In all the presented examples  $\mu$  was made as small as  $10^{-4}$ .

#### 4.4. Chemical engineering example: CSTR

Jacketed exothermic continuous stirred tank reactors (CSTRs) have been widely studied (Russo & Bequette, 1995) because of their challenging operational features and their outstanding importance in process industry. From Devia and Luyben (1978), the dynamics of a typical CSTR (Fig. 4) in which an homogeneous, exothermic, first order,  $A \rightarrow B$  reaction takes place, is described by the following set of equations:

$$\frac{dC_A}{dt} = \left(\frac{F}{V_R}\right)C_{A,0} - \left(\frac{F}{V_R}\right)C_A - C_A\alpha e^{-E/RT}$$

$$\frac{dT}{dt} = \left(\frac{F}{V_R}\right)T_0 - \left(\frac{F}{V_R}\right)T - \frac{\lambda C_A \alpha}{\rho C_p} e^{-E/RT} - \frac{UA_H}{\rho V_R C_p} \times (T - T_J)$$

$$\frac{dT_J}{dt} = \left(\frac{F_J}{V_J}\right)(T_{J,0} - T_J) + \frac{UA_H}{\rho_J C_J V_J} (T - T_J)$$

Table 1  
Optimization results of motivating example

c	p	$x_1$	$x_2$	$\lambda_1$	$\lambda_2$
0.90	0.287	-0.806	0.501	-0.607	-0.005
0.95	0.287	-0.653	0.724	-1.153+0.749i	-1.153-0.749i
1.00	0.287	-0.578	0.816	-0.077+0.850i	-0.077-0.850i
1.05	0.287	-0.513	0.887	-0.012+0.890i	-0.012-0.890i

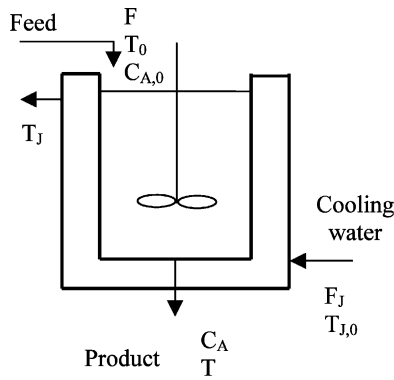


Fig. 4. Three states CSTR.

Reactor temperature ( $T$ ), reactant A concentration ( $C_A$ ) and cooling fluid temperature ( $T_j$ ) are the states of the system. The following restrictions should be considered in the design formulation because of geometric and operational reasons:

$$H_R = 2D_R$$

$$A_H = \pi D_R H_R + \frac{\pi}{4} D_R^2$$

$$V = \frac{\pi}{4} D_R^2 H_R$$

$$V_j = 0.25V$$

$$5 \leq D_R \leq 15$$

$$650 \leq T \leq 725$$

$$650 \leq T_j \leq 700$$

$$0 \leq C_A \leq 0.01$$

$D_R$ ,  $A_H$  and  $V_R$  stand for reactor diameter, reactor heat transfer area and reactor volume, respectively.  $V_j$  represents reactor jacket volume. Since heat transfer area is related to the square of the diameter, and reactor volume is related to the cubic of the diameter, certain designs may result unstable if enough heat-transfer capacity per unit volume is not achieved, as reported in Devia and Luyben (1978) for a number of cases. The proposed technique to ensure local dynamic stability in an uncertainty framework was applied to the design of the CSTR.

A typical total cost objective function to be minimized has been considered:

$$\text{Cost} = c_1 D_R^{1.066} H_R^{0.802} + c_2 F_j$$

The first term of the objective represents the capital cost, which depends on the size of the vessel according to a potential law. The second term stands for operating cost and is a linear function of the cooling utility. Productivity is not explicitly considered in the objective function since output reactant concentration is restricted

to be low and then high conversion is achieved in the reactor.

The design problem was solved for the numerical data of Table 2 and the following uncertainty realization:  $C_A$  (mol/cu. ft.) = {0.45, 0.50, 0.55},  $T_0$  (R) = {525, 530, 535}, and  $U$  (Btu/h per sq. ft. per R) = {145, 150, 155}. The proposed formulation was implemented in GAMS/rSQP and a reactor diameter  $D_r = 5.18$  ft. and cooling flow-rate,  $F_j = 45.44$  cu. ft./h were obtained as the design that is open-loop stable for the considered uncertainty and model constraints.

## 5. Optimal dynamic performance

Within the same philosophy, it is possible to formulate the design problem in order to optimize some sort of dynamic performance index. From Eq. (4) (let choose  $\mathbf{Q} = \mathbf{I}$ , as it is in general suggested) it can be seen that  $\eta = \lambda_{\min}(\mathbf{P}^{-1})$  becomes a natural objective function to be maximized in order to achieve a fast as possible transient response. Since  $\lambda_{\min}(\mathbf{P}^{-1}) = 1/\lambda_{\max}(\mathbf{P})$ , maximizing  $\lambda_{\min}(\mathbf{P}^{-1})$  corresponds to minimize  $\lambda_{\max}(\mathbf{P})$ , which is also a desirable objective in order to enlarge the estimate of the domain of attraction of the origin, as can be concluded from Eq. (3). Positive definite condition on matrix  $\mathbf{P}$  (or on  $\mathbf{P}^{-1}$ ) is also required. The resulting problem turns to become the following eigenvalue optimization, non-linear semi-definite programming problem:

$$\begin{aligned} & \min_y \lambda_{\max}(\mathbf{P}) \\ \text{s.t. } & \mathbf{A}(\mathbf{y}, \boldsymbol{\theta})^T \mathbf{P} + \mathbf{P} \mathbf{A}(\mathbf{y}, \boldsymbol{\theta}) + \mathbf{I} = \mathbf{0} \\ & \mathbf{P}^{-1} \succ \mathbf{0} \\ & \mathbf{h}(\mathbf{y}, \boldsymbol{\theta}) = \mathbf{0} \\ & \mathbf{g}(\mathbf{y}, \boldsymbol{\theta}) \leq \mathbf{0} \\ & \mathbf{y} \in \mathbf{Y}, \boldsymbol{\theta} \in \Omega \end{aligned} \quad (12)$$

By considering a slack variable  $z$ , which becomes an upper bound for the eigenvalues of  $\mathbf{P}$  (Ringertz, 1997), problem Eq. (12) may be posed as:

Table 2  
Numerical data

Feed flow-rate	F	50	cu. ft./h
Cooling water inlet temperature	$T_{j0}$	530	R
Reactor liquid heat capacity	$C_p$	0.75	Btu/lb. R
Jacket water heat capacity	$C_j$	1	Btu/lb. R
Reactor liquid density	$\rho$	50	lb/cu. ft.
Cooling water density	$\rho_j$	62.3	lb/cu. ft.
Pre-exponential factor	$\alpha$	7.08e10	1/hr
Activation energy	E	30 000	Btu/mol
Heat of reaction	$\lambda$	-30 000	Btu/mol
Cost coefficient 1	$C_1$	1917	
Cost coefficient 2	$C_2$	120	



$$\begin{aligned}
 & \min_{y,z} z \\
 \text{s.t.} & \mathbf{A}(y, \theta)^T \mathbf{P} + \mathbf{P}\mathbf{A}(y, \theta) + \mathbf{I} = \mathbf{0} \\
 & z > \lambda_i(\mathbf{P}), \quad i = 1, \dots, n \\
 & \lambda_i(\mathbf{P}^{-1}) > 0, \quad i = 1, \dots, n \\
 & \mathbf{h}(y, \theta) = \mathbf{0} \\
 & \mathbf{g}(y, \theta) \leq \mathbf{0} \\
 & y \in Y, \theta \in \Omega
 \end{aligned} \tag{13}$$

Again, this is a difficult non-smooth problem because of the eigenvalue constraints. Interior-point/logarithmic-barrier-transformation methods shown to be effective to tackle such problems as already commented. The barrier term corresponding to the  $z - \lambda_i(\mathbf{P}) > 0, i = 1, \dots, n$  constraints, may be posed as  $\sum_{i=1}^n \log(z - \lambda_i(\mathbf{P})) = \log[\prod_{i=1}^n (z - \lambda_i(\mathbf{P}))] = \log(\det(z\mathbf{I} - \mathbf{P}))$ . As already seen in the former sections, the barrier term for  $\lambda_i(\mathbf{P}^{-1}) > 0, i = 1, \dots, n$  is  $-\log(\det(\mathbf{P}))$ . Positive definiteness of both  $z\mathbf{I} - \mathbf{P}$  and  $\mathbf{P}$  should be verified at the solution as also commented. Problem Eq. (13) may then be reformulated as follows:

$$\begin{aligned}
 & \min_{y,z} \{z - \mu_1 \log(\det(z\mathbf{I} - \mathbf{P})) + \mu_2 \log(\det \mathbf{P})\} \\
 \text{s.t.} & \mathbf{A}(y, \theta)^T \mathbf{P} + \mathbf{P}\mathbf{A}(y, \theta) + \mathbf{I} = \mathbf{0} \\
 & \mathbf{h}(y, \theta) = \mathbf{0} \\
 & \mathbf{g}(y, \theta) \leq \mathbf{0} \\
 & y \in Y, \theta \in \Omega
 \end{aligned} \tag{14}$$

Again, from a feasible starting point, the solution of Eq. (14) converges to the solution of Eq. (13) for a decreasing sequence of barrier parameters  $\{\mu^k\}$  as  $\mu^k \rightarrow 0$ . The corresponding multi-period approximation is:

$$\begin{aligned}
 & \min_{y^i, z^i} \left\{ \sum_{i=1}^N z^i - \mu_1 \sum_{i=1}^N \log(\det(z^i \mathbf{I} - \mathbf{P}^i)) + \mu_2 \sum_{i=1}^N \log(\det(\mathbf{P}^i)) \right\} \\
 \text{s.t.} & \left. \begin{aligned} & \mathbf{A}^T(y^i, \theta^i) \mathbf{P}^i + \mathbf{P}^i \mathbf{A}(y^i, \theta^i) + \mathbf{I} = \mathbf{0} \\ & \mathbf{h}(y^i, \theta^i) = \mathbf{0} \\ & \mathbf{g}(y^i, \theta^i) \leq \mathbf{0} \end{aligned} \right\} \quad i = 1, \dots, N \tag{15}
 \end{aligned}$$

For our motivating example:

$$\begin{aligned}
 & \min \{z - \mu_1 \log(\det(z\mathbf{I} - \mathbf{P})) + \mu_2 \log(\det(\mathbf{P}))\} \\
 \text{s.t.} & \\
 & a_{11} = 2x_1 \\
 & a_{12} = 2x_2 \\
 & a_{21} = 2x_1 \\
 & a_{22} = 1 \\
 & 0 = 2a_{11}p_{11} + 2a_{21}p_{12} + 1 \\
 & 0 = a_{11}p_{12} + a_{21}p_{22} + a_{12}p_{11} + a_{22}p_{12} \\
 & 0 = 2a_{12}p_{12} + 2a_{22}p_{22} + 1 \\
 & \det(z\mathbf{I} - \mathbf{P}) = (z - p_{11})(z - p_{22}) - p_{12}^2 \\
 & \det(\mathbf{P}) = p_{11}p_{22} - p_{12}^2 \\
 & 0 = x_1^2 + x_2^2 - c \\
 & 0 = x_1^2 + x_2 - 4p
 \end{aligned}$$

$$\begin{aligned}
 & 0 \leq p \leq 1 \\
 & x_1 \leq 0 \\
 & x_2 \geq 0
 \end{aligned}$$

Parameter c realization is assumed to be  $\{0.90, 0.95, 1.00, 1.05\}$ , and the above model posed as Eq. (15). Table 3 summarizes the optimization results.

As expected, corresponding jacobian matrices are Hurwitz and then local stability verified for the proposed realization of uncertainty. The problem was solved with GAMS/CONOPT2.

The results reported in Table 3 are similar to those of Table 1 (both corresponding to the motivating example) for different objective functions. In the former model, however, the objective function value ( $\sum_0 x_2^2$ ) resulted in 2.2278 while the corresponding in the later is 2.238. From Table 3 it can be seen that  $\lambda_{\max}(\mathbf{P})$ , which is the objective to be minimized in the second case, is bounded by 177.76 while the corresponding to the previous model ( $\max\{\lambda_i(\mathbf{P})\}$ ) is 1928.2. These figures suggest the conflicting nature of the objectives, as expected in design problems between different performance indices, and determine a multiple objective design formulation. Multiple objective design is beyond the scope of this contribution but will be considered for future research.

### 5.1. Chemical engineering example: controller tuning of three non-interacting tanks

Such a design formulation appears to be well suited for feedback controller tuning, since a (closed-loop) dynamic performance index is optimized, and admits a straightforward approach to switchability by considering the set points as uncertain parameters. Again what we are trying to do is to ensure the existence of a certain domain of attraction for each point of the set-point realization as sketched in Fig. 5 for a two points set-point realization.

In order to illustrate this issue, the proportional feedback controller tuning of three non-interacting tanks in series (extended model from Ogunnaike & Ray, 1994) (Fig. 6), will be performed in the following. Although the system is open-loop stable, an overly aggressive control action (controller gain too large) may drive the system to closed-loop instability. The following dynamic model is considered:

$$\begin{aligned}
 \frac{dh_1}{dt} &= -\frac{1}{\tau_1} \sqrt{h_1} + \frac{K_1}{\tau_1} F_0 \\
 \frac{dh_2}{dt} &= \frac{K_2}{\tau_2} \sqrt{h_1} - \frac{1}{\tau_2} \sqrt{h_2} \\
 \frac{dh_3}{dt} &= \frac{K_3}{\tau_3} \sqrt{h_2} - \frac{1}{\tau_3} \sqrt{h_3} \\
 F_0 &= K_c(h_{3sp} - h_3) + F_{0sp}
 \end{aligned}$$

Table 3  
Optimization results of motivating example

c	p	z	$x_1$	$x_2$	$\lambda_1$	$\lambda_2$
0.90	0.287	177.76	-0.800	0.511	-0.534	-0.066
0.95	0.287	177.76	-0.653	0.724	-1.153+0.749i	-1.153-0.749i
1.00	0.287	177.76	-0.577	0.816	-0.077+0.850i	-0.077-0.850i
1.05	0.287	177.76	-0.512	0.887	-0.012+0.890i	-0.012-0.890i

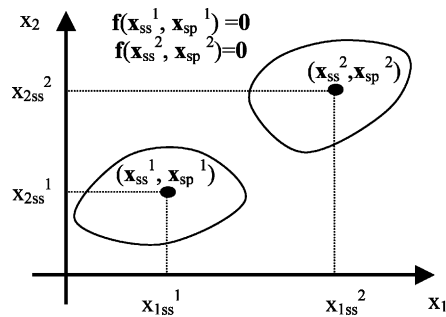


Fig. 5. Local stability for set-point changes.

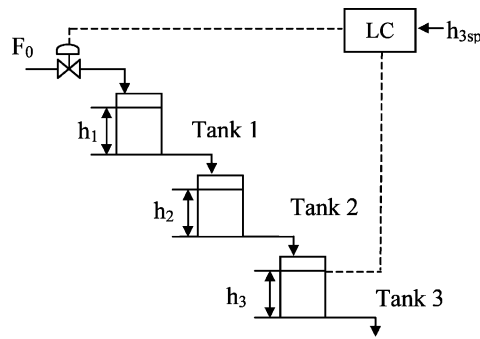


Fig. 6. Three non-interacting tanks in series.

$h_i$  stands for tank level,  $K_c$  is the proportional controller gain and subscript sp corresponds to set-point value. Numerical data are presented in Table 4.

Steady-state open-loop values for the levels are  $h_1 = 0.25$ ,  $h_2 = 1.00$  and  $h_3 = 9.00$ . In order to consider the switchability issue, the following realization is considered for  $h_{3sp}$ :  $\{7.00, 8.00, 9.00, 10.00, 11.00\}$ . A Eq. (15) type formulation was solved for the above model and

Table 4  
Data for non-interacting tanks system

$\tau_1$	2
$\tau_2$	4
$\tau_3$	6
$K_1$	1
$K_2$	2
$K_3$	3
$F_{0sp}$	0.5

data with GAMS/CONOPT2. Results are summarized in Table 5.

The corresponding eigenstructure for the considered set point realization is graphically shown in Fig. 7. As expected the eigenvalues remain in the stable part of the complex space although closer to critical stability as  $h_{3sp}$  increases. The inclusion of stability margins, as suggested in Ringertz (1997) and commented previously for the motivating example, is not obvious and remain an issue for future research.

## 6. Conclusions

In this paper, we have presented a new theoretical formulation for the problem of interaction between process design and process operability, approaching the controllability/switchability issue within an eigenvalue optimization framework. The proposed technique allows the generation of economically optimal open-loop designs, which are also locally dynamically stable in a Lyapunov's sense. The problem of control tuning has been also addressed, by optimizing a dynamical performance index related to convergence response speed: the minimum eigenvalue of matrix  $\mathbf{P}^{-1}$ , which is desired to be maximized. The new framework also avoid the use of dynamic simulation at the process design stage, relying entirely on steady-state formulations to simultaneously consider design and operability.

To consider flexibility in the face of parametric and disturbance uncertainty, a deterministic-based approximation, that gives rise a multi-period program by defining in advance a certain realization of uncertainty, has been applied. Future work will take into account the application of energy function techniques to the assessment of non-linear behavior through the analysis of the

Table 5  
Optimization results for non-interacting tanks system

$h_{3sp}$	z	$K_c$	$h_1$	$h_2$	$h_3$
7	28.14	0.26	0.15	0.61	5.48
8	28.14	0.26	0.18	0.71	6.36
9	28.14	0.26	0.20	0.81	7.24
10	28.14	0.26	0.23	0.91	8.14
11	28.14	0.26	0.25	1.00	9.00

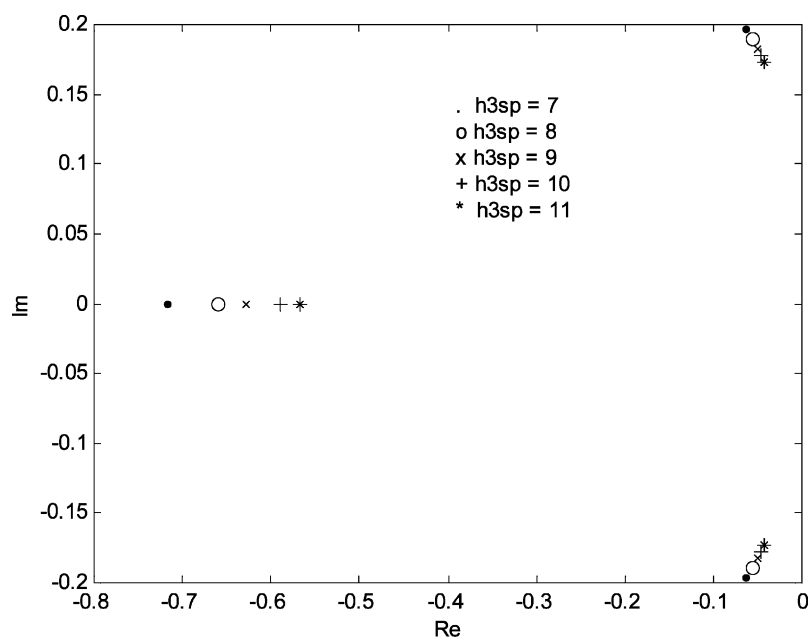


Fig. 7. Eigenstructure for the set-point realization of the three non-interacting tanks in series.

shape and size of the domains of attraction of the equilibrium points. The trade-off between economics and dynamic performance, which may be naturally posed as a multi-objective optimization problem, will also be explored.

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