A Robust Dynamic Feasibility Analysis for the Simultaneous Design and Control of Dynamic Systems under Uncertainty

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Abstract: This paper presents a new simultaneous design and control approach that considers flowsheet synthesis and control structure selection. The key idea on this work is to estimate the worst-case variability in the dynamic feasibility constraints from simulations of the closed-loop process model using the worst-case realization in the disturbances. The critical disturbance profile is obtained from a robust performance formulation based on Structured Singular Value ($\mu$) analysis. The proposed approach reduces the computational time of the calculations because dynamic optimization is not required in the dynamic feasibility test. A system of reactors in series is used to test the proposed simultaneous design and control methodology.

Keywords: Design and control, control systems design, structural optimization, structured singular value.

1. INTRODUCTION

Integration of process design and control searches for the optimal process design and control configuration by considering both the steady-state and the dynamic operation of the process in closed-loop, in the presence of external perturbations and uncertainties in the process parameters. Due to its complexity, only a few simultaneous design and control methodologies that consider structural changes in the formulation have been developed (Mohideen et al. 1996; Bahri et al. 1997; Malcom et al. 2007; Kookos and Perkins 2001; Seferlis and Grievink 2004). Most of these methodologies decompose the problem into a dynamic flexibility analysis and a dynamic feasibility test. While the dynamic flexibility analysis searches for the optimal design and control configuration in the presence of specific time-varying realizations in the disturbances, the dynamic feasibility test ensures that the optimal design and control scheme, found in the previous step, comply with the process feasibility constraints in the presence of critical realizations in the disturbance. That is, the feasibility test searches for that critical time-varying profile in the perturbations that produces the largest variability in the process feasibility constraints. The current methodologies that perform integration of design and control formulate the feasibility test as a nonlinear dynamic optimization problem, which is computationally demanding even for simple dynamic systems. Also, most of the methodologies available assume that the critical time-varying profile in the disturbance can be represented as a pre-specified function with unknown parameters. The known (critical) parameters of these functions that produce the worst-case variation in the feasibility constraints are obtained by running extensive simulations of the mechanistic closed-loop process model in the dynamic feasibility test. Thus, the optimal design and control configuration obtained by these methods is only valid for critical disturbances that follow the dynamic behaviour of the pre-specified function. That is, there is no guarantee that other worst-case disturbance realizations with a different time-dependent profile may violate the process feasibility constraints.

This paper presents a new simultaneous design and control methodology that considers structural decisions in the formulation. The key idea in this work is to propose a robust dynamic feasibility test that estimates the critical realizations in the disturbance that produces the largest deviation in the process feasibility constraints. The proposed approach does not make any assumptions about the disturbance dynamics, as was the case in previous methodologies. That is, the disturbance is treated here as a time-varying magnitude-bounded perturbation. The proposed feasibility test is based on a robust performance tool formulated as a convex optimization problem. Thus, the proposed feasibility test is computationally attractive because it does not require the solution of a dynamic optimization problem.

2. METHODOLOGY

This section presents the approach proposed to simultaneously design and control dynamic systems that consider flowsheet synthesis and control structure selection. Fig. 1 shows the iterative decomposition algorithm proposed for this methodology. As shown in the Figure, the simultaneous design and control formulation is decomposed in a closed-loop dynamic flexibility analysis and a robust dynamic feasibility test. This decomposition approach has been the preferred method for solving simultaneous design and control problems that involve structural decision in the analysis. While the dynamic flexibility analysis used in this work is similar to that proposed by other methodologies (Bahri et al. 1997; Mohideen et al., 1996, Kookos and Perkins, 2001), a new robust approach is presented here for the dynamic feasibility test. The details of each of these problems are discussed next.
2.1 Dynamic flexibility analysis

The first step in the iterative approach is to search for the process flowsheet, the control structure, the size of the units, the controller tuning parameters, and the set points that minimize a cost function (F) and satisfy the process constraints for a specific time-dependent profile in the disturbance at the kth iteration, v_k. This problem, usually referred to as a dynamic flexibility analysis, is mathematically described in problem (1). The terms x and h represent the state variables of the process and the controller equations, respectively; g represents the set of manipulated variables whereas the optimization variable u represents the remaining process variables that are set to a nominal operating value, e.g. set points. Likewise, d represents the continuous design variables, e.g. the size of a tank, whereas θ and Ω represent binary decisions that account for structural changes in the design of the process and in the control configuration, respectively. The functions f_m, f_c, and f_d represent the process model equations, the controller equations and the process feasibility constraints, respectively. The specific disturbance profile at the k-th iteration (v_k) remains unchanged throughout the solution of problem (1). Consequently, the design and control scheme obtained from (1) are only valid for that profile in v_k. Problem (1) can be classified as an infinite mixed-integer nonlinear dynamic optimization problem. Several approaches have been proposed to solve this problem within the context of integration of design and control, e.g. Mohideen et al. 1996, Bahri et al. 1997, Malcom et al. 2007. In the current work, a numerical integration approach was used to perform the dynamic flexibility analysis. At each optimization step, the closed-loop mechanistic process model is simulated using v_k as an input. The simulation results are used to evaluate the constraints (f_d) and the cost function (F). The results obtained from these evaluations are used to select new values in the decision variables for the next iteration in the optimization. This procedure continues until an optimization criterion is met. To solve problem (1), the set of those process flowsheets and control structures that promises to be an optimal solution need to be considered in the analysis. Often, the promising process flowsheets and control structures are embedded in a single representation known as the superstructure. This superstructure is mathematically defined by the different combinations between the binary optimization variables θ and Ω, respectively. The construction of the superstructure is given elsewhere, e.g., Kocis and Grossmann (1989).

\[
\begin{align*}
\min & \quad F \\
\text{s.t.} & \quad f_m(x(t), d, u, \theta, v_k(t), x(t), g(t)) = 0, \quad f_c(x(t), d, u, \theta, v_k(t), x(t), h(t), g(t)) = 0, \quad f_d(x(t), d, u, \theta, v_k(t), x(t), h(t), g(t)) \leq 0, \quad f_j(t) \in F_j \\
& \quad t \in [0, t_f] \\
\end{align*}
\]

where

\[
\begin{align*}
& d = [d_1, d_2 \leq \ldots \leq d_n] \\
& \lambda = [\lambda_1, \lambda_2 \leq \ldots \leq \lambda_m] \\
& u = [u_1, u_2 \leq \ldots \leq u_n] \\
& v_k(t) = [v_{k1}(t), v_{k2}(t) \leq \ldots \leq v_{kn}(t)] \\
& g(t) = [g_1(t), g_2(t) \leq \ldots \leq g_m(t)] \\
& \theta = [\theta_1, \theta \in [0,1]] \\
& \Omega = [\Omega_1, \Omega \in [0,1]] \\
\end{align*}
\]

2.2 Robust dynamic feasibility test

The design and control configuration obtained from the dynamic flexibility analysis at the kth iteration is only valid for a particular realization in v_k. Thus, a dynamic feasibility test is required to ensure that other critical realizations in the disturbance comply with the feasibility constraints considered in (1). The solution of this problem is computationally challenging because one must search for the disturbance profile, v_k, formed by individual realizations in the disturbance at a given time interval, that produce the worst-case variability in the feasibility constraints. To reduce the computational effort, previous methodologies have assumed that the critical disturbance profile follows a particular time-dependent function with unknown parameters. Thus, the dynamic feasibility test searches only for the critical parameters in those functions, e.g. the magnitude of a step change (Bahri et al. 1997) or the amplitude and/or frequency of a sinusoidal function (Kookos and Perkins, 2001), that may cause a violation in the process constraints.

In the present work, a new approach is presented for the dynamic feasibility analysis. The key idea on this approach is to estimate the critical time-dependent realizations in v_k that generate the maximum deviation in the feasibility constraints at any time, t, using a robust performance tool based on Structured Singular Value (μ) analysis. This robust tool (3) calculates bounds on the largest variability of a process
variable, e.g., \( y \), due to the worst-case realizations in the disturbances. The optimization parameter \( y' \) in (3) denotes a bound on the worst-case realization in the process variable \( y \). The matrices \( M \) and \( \Delta \) shown in (3) are the nominal matrix and the perturbation block in the \( \mu \) analysis calculation. The construction of these matrices is given in Ricardo-Sandoval et al. (2010).

\[
\max_{y'} \gamma' \\
\text{s.t.} \quad \mu(M) \leq \\frac{\gamma'}{\gamma}
\]  
(3)

To estimate \( y' \), problem (3) requires the specification of the maximum absolute deviation in the \( q^a \) disturbance \( \delta v_q \) at any time \( t \), which is obtained from the difference between the upper and lower limits specified for that particular disturbance, i.e., \( \delta v_q = |q_{\max} - q_{\min}| \). To account for the process dynamics, the robust formulation in (3) also requires the identification of an Uncertain Closed-loop Finite Impulse Response (UCFIR) model that describes the transient behaviour of the mechanistic closed-loop process model. To obtain an UCFIR model, the closed-loop mechanistic process model, i.e., the nonlinear process model equations \( (F_u) \) and the controller equations \( (F_c) \) considered in (1), is simulated using, as input, an excitation signal in the disturbance. The dynamic simulations are performed around a nominal operating point defined by \( d^*, u^*, 0* \) and \( \Omega^* \), which are the optimal parameters obtained from the solution of (1). Accordingly, the UCFIR model is only valid around that operating point. The data collected from the dynamic simulations is used to estimate the UCFIR model parameters using an identification technique, i.e., least-squares. The identified UCFIR model is as follows:

\[
y = \sum_{n=1}^{N} \sum_{a=1}^{Q}(s_n + \delta s_n) v_{\delta}(N-n)
\]  
(4)

where \( y \) represents a time-varying process variable used in the evaluation of the process feasibility constraints, e.g., \( f_f \), in (1). The parameter \( s_n \) represents the nominal impulse response coefficients obtained from the identification process whereas \( \delta s_n \) represents the uncertainty associated with the nominal impulse response parameters, which are assumed to be the variance of the linear model estimates. The variance of the least-squares parameters may be obtained from the covariance matrix of the model parameter estimates generated during the least-squares identification process. The uncertain model parameters, \( \delta s_n \), are included in (4) to account for the closed-loop process nonlinearities due to changes in \( v_q \). The term \( v_{\delta}(N-n) \) represent the deviations of the \( q^a \) disturbance at time \( N-n \) where \( N \) represents the closed-loop process settling time. Note that \( v_{\delta}(N-n) \leq \delta v_q \) and that the disturbance set \( (v) \) may contain \( Q \) disturbances. The conservatism associated with the UCFIR model depends on the degree of nonlinearity of the mechanistic process model. Since the UCFIR model is identified in closed-loop around a nominal operating condition, it is expected that the process oscillates around a nominal operation condition thus making the system behave as somewhat of a linear model. Hence, the uncertain model parameters \( (\delta s_n) \) are expected to be small. Although \( \delta v_q, s_n \) and \( \delta s_n \) are not explicitly shown in (3), they are the key parameters in building the nominal matrix \( (M) \) and the perturbation block \( (\Delta) \) in (3), respectively. The \( \mu \) analysis calculation searches for the elements in \( \Delta \) that makes \( \det(I-M \Delta) = 0 \) (Doyle, 1982). The elements of \( \Delta \) that describe the sources of uncertainty in (3) are \( \delta s_n \) and \( \delta v_q \), respectively. Thus, the solution to problem (3) returns the bound \( y' \) on the worst-case variability for \( y \) and the combination in the elements of \( \Delta \) that produces this critical scenario. Consequently, the critical disturbance profiles that produce the worst-case variability in \( y \) are also obtained from this calculation. Thus, the critical realizations in the disturbance, extracted from \( \Delta \) at the solution, can be used as inputs to simulate the closed-loop mechanistic process model to obtain the actual worst-case variability in \( y \). While (3) returns the worst-case disturbance vector that produces the maximum variability of \( y \) in the positive direction \( (y_{\max}^+) \), the negative of this worst-case disturbance vector returns the maximum variability in \( y \) in the negative direction \( (y_{\max}^-) \). Note that problem (3) is a convex optimization problem (Doyle, 1982) that can be solved using computationally efficient optimization algorithms. This represents a key advantage in the present approach since the calculation of the worst-case disturbance is performed quickly when compared to the challenging task of obtaining this critical profile from dynamic optimization. Thus, the robust tool shown in (3) is used by the present analysis to test the dynamic feasibility constraints. The mathematical description of the robust dynamic feasibility test is as follows:

\[
\Phi_k = \max_{x \in \mathbb{R}^k} \chi_k \\
\text{s.t.} \quad \chi_{ij} = f_{jx} + f_{jy}^{*}
\]  
(5)

where \( f_{jx} \) represents the \( j^\mu \) process constraint evaluated at steady-state, i.e.,

\[
f_{jx}(d^*, u^*, 0^*, \Omega^*, v_{\delta}, x_{\delta}, h_{\delta}, g_{\delta}) \leq 0
\]  
(6)

where the subscript ‘\( \mu \)’ denote a nominal condition for the time-dependent variables. The function \( f_{jy}^{*} \) in (5) represents the maximum deviation in the \( j^\mu \) process feasibility constraint, which is estimated from simulations of the mechanistic closed-loop process model using the worst-case disturbance profile obtained from (3). Note that \( \Phi_k \) in (5) is a scalar. As shown in Fig. 1, a negative \( \Phi_k \) indicates that the process constraints considered in the design and control formulation remain feasible in the presence of critical realizations in the disturbance \( (v_{\delta}) \). Thus, the design and control configuration obtained from the dynamic flexibility analysis (1) at the \( k^{th} \) iteration represent an optimal solution to this problem and the algorithm is terminated. On the other hand, a positive \( \Phi_k \) indicates that at least one process constraint exceeds its limits. Thus, the critical disturbance vector \( v_{\delta} \) is updated with the vector that produced the constraint violation in the feasibility test and it is used to rerun the dynamic flexibility test in the next iteration. This iterative procedure continues up until a maximum number of iterations are reached or a negative \( \Phi_k \) is obtained from the robust feasibility test.

### 3. CASE STUDY: A SYSTEM OF CSTR’S IN SERIES

The methodology presented in the previous section was applied to a system of reactors in series. Fig. 2 shows the
process superstructure composed of two continuous stirred tank reactors (CSTR) connected in series.

Fig. 2. Process superstructure

An exothermic, irreversible reaction that transforms reactant A into product B takes place in both reactors, i.e., A→B. The inlet stream flowrate, \( q_f(t) \), fluctuates between lower and upper limits due to time-varying changes in the upstream process. Thus, this variable is assumed to be the disturbance (\( v \)) for this process and is described as follows:

\[
q_f = [q_f(t) | 70 \text{L/min} \leq q_f(t) \leq 230 \text{L/min}] \tag{7}
\]

That is, \( q_f \) can take any value between its upper and lower limits during the continuous operation of this process. The minimum and maximum allowed temperatures on each reactor are as follows:

\[
400K \leq T_i(t) \leq 500K, \ i=1,2 \tag{8}
\]

where the subscript \( i \) indicates the CSTR unit. The goal for this process is to produce a stream with a concentration in reactant A that should not exceed 0.05 mol/L during the continuous operation of the system, i.e., produce a stream with high content in product B. To satisfy this requirement, the following constraint was included in the analysis:

\[
C_{A,i}(t) \leq 0.05 \quad P \in [1,2] \tag{9}
\]

where \( C_{A,i}(t) \) represents the variations in time of the concentration of component A in the product stream \( P \). The design and control scheme defined for this process should meet the purity specifications and satisfy the reactors’ temperature constraints in the presence of random fluctuations in \( q_f \). According to the superstructure defined for this process, only one CSTR may be needed to achieve the process goals, i.e., \( i=1 \) and \( P=1 \) in (8)-(9), whereas \( i=1,2 \) and \( P=2 \) in (8)-(9) are specified when two CSTR’s are used. The mechanistic process model for this system is shown in (10). The parameter \( D \) is a binary optimization variable that chooses between one or two CSTR units whereas \( R \) is a continuous variable (0≤\( R \)≤1) used to distribute the feed flowrate between the CSTR units (see Fig. 2). Following (10), \( T_F \) is the input streams’ temperature (350 K), \( k_o \) is the pre-exponential factor (7.2e-10), \( E \) is the activation energy (83145 J/mol), \( R \) is the gas constant (8.3144 J/mol-K), \( \rho \) is the fluid’s density (1e3 g/L), \( C_p \) is the fluid’s heat capacity (0.239 J/g-K) and \( \Delta H_R \) is the heat of reaction (4.78e4 J/mol).

\[
\begin{align*}
V_1 &= q_{F1} - q_1 \\
T_1 &= q_{F1}(T_F - T_i)/V_1 \\
+ \Delta H_R C_{A1} \exp\left(\frac{-E}{RT_1}\right)/\rho C_p - Q_{C1} \\
\dot{C}_{A1} &= q_{F1}(C_{A,F1} - C_{A1})/V_1 - k_0 C_{A1} \exp\left(\frac{-E}{RT_1}\right) \\
V_2 &= D(q_{F2} + q_2 - q_3) \\
T_2 &= q_{F2}(T_F - T_2)/V_2 + q_1(T_1 - T_2)/V_2 \\
+ \Delta H_R C_{A2} \exp\left(\frac{-E}{RT_2}\right)/\rho C_p - Q_{C2} \\
\dot{C}_{A2} &= D(q_{F2}(C_{A,F2} - C_{A2}))/V_2 \\
+ q_1(C_{A1}(C_{A,F2}))/V_2 - k_0 C_{A2} \exp\left(\frac{-E}{RT_2}\right) \\
Q_{C1} &= 48.1909 g_1 \\
q_1 &= 10g_1\sqrt{V_1} \\
Q_{C2} &= 48.1909 g_3 \\
q_2 &= 10g_1\sqrt{V_2} \\
q_{F3} &= q_F(1 - RD) \\
q_{F2} &= q_F RD \tag{10}
\end{align*}
\]

The present analysis considers three potential process design configurations: i) A single CSTR with a single feed stream \( q_{F1} \), \( D=0 \) and \( R=0 \), ii) Two CSTR’s with one feed stream for the first reactor \( q_{F1} \) and two feed streams for the second reactor, \( q_1 \) and \( q_2 \), i.e., \( D=1, R=0 \), and iii) Two CSTR’s with one feed stream for the first reactor \( q_{F1} \) and one feed stream for the second reactor \( q_2 \), i.e., \( D=1 \) and \( R=0 \). The temperature, volume and concentration on each CSTR, i.e., \( T_F, V_1, C_{A1}, T_2, V_2, C_{A2} \), are assumed to be measured online whereas the volumetric flowrate at the outlet of each unit, \( q_1 \) and \( q_2 \), and the cooling heat flow on each reactor, \( Q_{C1} \) and \( Q_{C2} \), are assumed to be adjustable variables available for control. Thus, there are 6 potential controlled variables (CV’s) and 4 manipulated variables (MV’s) for this process. A set of decentralized multi-loop control structures was considered as the control superstructure for this system. As shown in (11), the control superstructure considers feedback controllers of type Proportional-Integral (PI).

\[
\begin{align*}
\dot{I}_{im} &= \Omega_{im} \left( e_{im} \right) \\
\gamma_{im} &= \Omega_{im} \left( \sigma_{im} + KC_{im} \left( e_{im} + I_{im} \right) \right) \\
e_{im} &= y_{im} - \gamma_{im} \\
\sum_{i=1}^{3} \sum_{j=1}^{3} \Omega_{im} \leq 1, & \quad \sum_{i=4}^{6} \sum_{j=4}^{6} \sum_{l=1}^{3} D\Omega_{im} \leq 1 \\
\sum_{i=1}^{3} \sum_{j=1}^{3} \Omega_{im} \leq 1, & \quad \sum_{i=4}^{6} \sum_{j=4}^{6} \sum_{l=4}^{6} D\Omega_{im} \leq 1
\end{align*}
\]

The term \( e_{im} \) in (11) represents the errors between the set point \( y_{im} \) and the measurement \( \gamma_{im} \) when the \( i^{th} \) MV is used to control the \( m^{th} \) CV. The term \( \Omega_{im} \) is a binary optimization variable that specifies the pairing between the \( i^{th} \) MV and the \( m^{th} \) CV. The set of \( \Omega_{im} \), \( \Omega \), defines the decentralized control structure for this system. The logical
constraints in (11) ensure that the multi-loop control structure selected is feasible. The PI controller tuning parameters for each control loop considered in the control superstructure ($K_{C \text{in}}$ and $T_{\text{in}}$) are also considered as optimization variables in the formulation. The term $I_{\text{in}}$ denotes the controller states for each control loop whereas $g_{\text{in}}$ and $\sigma_{\text{in}}$ represent the actual and the nominal values in the $i^{th}$ MV paired with the $m^{th}$ CV.

3.1 Dynamic flexibility analysis

The annualized cost function proposed for this system ($\Gamma_{CS}$) is shown in (12). The annualized capital cost function ($CC_{CS}$) was defined in terms of the capacities required for each CSTR. Each reactor was assumed to be a pressurized vessel of height $H_i$ and diameter $Diam_i$. The dimensions of each CSTR were calculated using the maximum liquid holdup variability ($V_{\text{max}}$), that is estimated from simulations of the mechanistic closed-loop process model using, as input, the critical realizations in the disturbance $\Phi$. The term $r$ in $CC_{CS}$ represents the annualized rate of return ($r=0.1$).

$$
\Gamma_{CS} = CC_{CS} + OP_{CS} + VC_{CS}
$$

$$
CC_{CS} = 1917(\text{Diam}_i^{1.066}H_i^{0.802} + DD\text{iam}_i^{1.066}H_i^{0.802})
$$

$$
Diam_i = \left(0.03532V_{\text{max}}^*/4\pi\right)^{1/2}, \quad i = 1,2
$$

$$
H_i = \left(0.03532V_{\text{max}}^*/4\pi\right)^{1/4}, \quad i = 1,2
$$

$$
OP_{CS} = 8.76E_{c}\left(Q_{1,\phi} + DQ_{2,\phi}\right)
$$

$$
VC_{CS} = 5.256\times10^5 \beta w_{A,P,\text{max}}^*
$$

Following (12), the energy consumption considered in the operating cost function ($OP_{CS}$) was measured in terms of the cooling heat rates, $Q_{\phi}$, and $Q_{\phi}$, required by the units. The term $E_{c}$ ($\$3.8$/kW-h)$ represents the energy costs assigned to $Q_{\phi}$ and $Q_{\phi}$, respectively. The variability cost ($VC_{CS}$) is a function that measures the dynamic performance of the closed-loop system in the presence of critical realizations in the disturbance, $\Phi$. The variability function is process-specific and is defined in terms of the goals to attain by the design and control configuration. In the present analysis, the variability cost function was defined as a function of the worst-case variability in the composition of A in the product’s stream. As shown in (12), the parameter $\beta$ ($\$0.001$/mol of A) is a cost assigned to the maximum molar flowrate variability expected for reactant A in the product’s stream ($w_{A,P,\text{max}}^*$). That is, the dynamic performance of the plant was measured in terms of the ability of the design and control scheme to keep A’s molar flowrate in the product’s stream ($w_{A,P}$) to the minimum in the presence of the worst-case variation in $\Phi$. The larger the molar flowrate of A in the product’s stream, the larger the variability costs assigned to the system. The constant terms in $OP_{CS}$ and $VC_{CS}$ are conversion factors. Note that $D$ is included in (12) to account for structural changes in the design.

Problem (1) was reformulated in terms of the cost function (12), the mechanistic process model (10), the decentralized control superstructure (11) and the process constraints (8)-(9), to define the dynamic flexibility analysis for this system. The optimization variables for this problem are the binary variable $D$, that selects the process design structure ($\theta$ in problem 1); the set of $\Omega$ that defines the control structure; a set of 24 controller tuning parameters ($\lambda$, in problem 1), i.e. $K_{C \text{in}}$ and $T_{\text{in}}$; the continuous parameter $R$; the set points for the temperature on each reactor ($T_{i}$ and $\bar{T}_{i}$), and the nominal concentration of component A in the product’s stream, $C_{A,P}$. The maximum and minimum variability in the reactor’s temperature ($T_{i,\text{max}}^*$ and $T_{i,\text{min}}^*$) and the maximum concentration of A in the product’s stream ($C_{A,P,\text{max}}^*$) were used to evaluate the temperature and concentration constraints shown in (8) and (9), respectively. These extreme values were obtained from simulations of the closed-loop mechanistic process model using, as input, the critical realizations in $\Phi$. The dynamic flexibility analysis for this system was solved using the numerical integration approach described in section 2.1.

3.2 Robust dynamic feasibility test

The robust feasibility test shown in (5) was reformulated, according to the specifications given for this case study, and is described as follows:

$$
\Phi_{\text{ACS}} = \max_{\Phi_{\text{ACS}}} \chi_{\Phi_{\text{ACS}}}
$$

$$
\begin{align*}
\chi_{\Phi_{\text{ACS}}} \Delta T_{1} & = T_{\text{in}}^* - T_{\text{in,\text{max}}} - 500 \\
\chi_{\Phi_{\text{ACS}}} \Delta T_{2} & = T_{\text{in}}^* - T_{\text{in,\text{min}}} - 400 \\
\chi_{\Phi_{\text{ACS}}} \Delta T_{3} & = D(T_{\text{in}}^* - T_{\text{in,\text{max}}} - 500) \\
\chi_{\Phi_{\text{ACS}}} \Delta T_{4} & = D(T_{\text{in}}^* - T_{\text{in,\text{min}}} - 400) \\
\chi_{\Phi_{\text{ACS}}} \Delta T_{5} & = (1 - D)(\hat{C}_{A,1}^* + C_{A,\text{\text{max}}}^* - 0.05) \\
\chi_{\Phi_{\text{ACS}}} \Delta T_{6} & = D(\hat{C}_{A,2}^* + C_{A,\text{\text{max}}}^* - 0.05)
\end{align*}
$$

where the process variables with the superscript $\gamma^*$ represent the worst-case variability on these variables due to the worst-case realization in the inlet stream flowrate, $\Phi$. The worst-case variability in the process variables is obtained from simulations of the mechanistic closed-loop process model using the worst-case profile in $\Phi$, which is obtained from the robust performance calculation shown in (3). To compute the worst-case variability, UCFIR models from $\Phi$ to $T_{i}$, $C_{A,i}$, are identified when the solution from the dynamic flexibility test specifies $D=0$ (flowsheet with a single CSTR) whereas UCFIR models from $\Phi$ to $T_{i}$, $T_{i}$, and $C_{A,i}$, are required when the dynamic flexibility analysis returns $D=1$ (flowsheet with two CSTR’s). The simultaneous design and control formulation proposed for this case study was solved in MATLAB. The dynamic flexibility test was solved using the glcDirect solver available in the TOMLAB toolbox that solves MINLP. The convex optimization problem shown in (3) was solved using the fmincon built-in function available in MATLAB. The initial disturbance profile used in the dynamic flexibility analysis ($\Phi_{\Phi}$ in Fig. 1) was assumed to be a step change in the inlet stream flowrate from 170 to 230 L/min. Table 1 summarizes the design and control configuration obtained for this case study (Flowsheet synthesis). As shown on this Table, two CSTR’s and three feedback control loops are required to maintain the feasible
operation of the system in the presence of the worst-case realization in \( q_F \). To analyze the effect of structural changes on the optimization results, the simultaneous design and control of a single CSTR was considered. That is, the process flowsheet was fixed \((D=0 \text{ and } R=0 \text{ in 10, 11 and 13}) \) and the control structure was selected according to (12) for a single process unit. As shown in Table 1 (Flowsheet fixed), a single CSTR with two control PI loops can also achieve the design and control goals specified for this system. However, the annualized costs estimated for that design and control scheme are more than double the costs obtained when flowsheet synthesis was considered in the analysis. This result confirms that the proposed approach for the simultaneous selection of the process flowsheet and the control structure returns optimally integrated plants that satisfy the dynamic feasibility constraints in the presence of critical variations in the perturbations. To validate the results for flowsheet synthesis formulation, the design and control scheme was simulated using the worst-case disturbance profile obtained from the robust dynamic feasibility test at the last iteration step. Fig. 3 shows that the worst-case disturbance profile is not trivial. Thus, it would be challenging to obtain this profile using pre-specified functions as it has been proposed in previous simultaneous design and control methodologies. Fig. 4 shows that the concentration of A in the product’s stream remains within the desired design specifications, when the critical profile in \( q_F \) is used to simulate the design and control configuration obtained by the present method. The rest of the constraints in (13) were also validated using the same procedure. Therefore, the design and control scheme found by the present formulation achieves the design and control goals at minimum cost and satisfies the feasibility constraints in the presence of the worst-case disturbance. The design and control scheme obtained for the single CSTR case study was also validated but it is not shown here for brevity.

### Table 1. Optimal design and control configuration

<table>
<thead>
<tr>
<th>Variable</th>
<th>Flowsheet synthesis</th>
<th>Flowsheet fixed</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>1.0</td>
<td>0.0 (fixed)</td>
</tr>
<tr>
<td>R</td>
<td>0.25</td>
<td>0.0 (fixed)</td>
</tr>
<tr>
<td>( \dot{F}_1 ) (K)</td>
<td>484.0</td>
<td>499.0</td>
</tr>
<tr>
<td>( \dot{F}_2 ) (K)</td>
<td>484.0</td>
<td>--</td>
</tr>
<tr>
<td>( C_{A,P} ) (mol/L)</td>
<td>0.010</td>
<td>0.012</td>
</tr>
<tr>
<td>Control loop 1</td>
<td>( q_1-V_1 )</td>
<td>( q_1-V_1 )</td>
</tr>
<tr>
<td>Control loop 2</td>
<td>( q_2-V_2 )</td>
<td>( q_2-T_1 )</td>
</tr>
<tr>
<td>Control loop 3</td>
<td>( Q_{CS}-C_{A,2} )</td>
<td>--</td>
</tr>
<tr>
<td>( T_{CS} ) (S/yr)</td>
<td>34,931.00</td>
<td>73,776.71</td>
</tr>
</tbody>
</table>

Fig. 3. Worst-case realization in the disturbance

Fig. 4. Worst-case variability in \( C_{A,P} (P=2) \)

### 4. CONCLUSIONS

A new robust simultaneous design and control methodology that takes into account structural decisions in the analysis has been presented. The key idea of this work is to propose a robust dynamic feasibility test that calculates the worst-case variability on the feasibility constraints for a fixed design and control scheme. The worst-case variability is obtained from a robust tool defined as a convex optimization problem, i.e., the proposed approach is computationally efficient. Current work in this area considers the use of model-based controllers within the method, e.g. MPC or Q-parameterization, and the development of a new approach that reduces the computational effort in the dynamic flexibility analysis.

### ACKNOWLEDGEMENTS

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### REFERENCES


