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Efficient feasible set characterization through Distance Field Map algorithm and its use in control ⋆

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Abstract: The feasibility of processes is a well-used notion with several definitions in the literature according to each context. This is understood as the region of operative variables where phenomena of processes occur. In this work, we propose a definition for the feasibility set and explain an algorithm to characterize efficiently its shape and size. Additionally, we define a feasibility index to quantify the belonging grade of a point inside the feasible set, instead of the yes/no usual belonging function. Finally, this paper shows the use of previous concepts for control proposes. In an example, we found the set-point for a process through an optimization problem, guaranteeing the feasibility in the presence of disturbances and improving its productivity.

Keywords: Feasible set, optimization, Medial axis, Distance Field Map

1. INTRODUCTION

Economical goals determine generally the operation of processes: to increase productivity, to improve the quality of products, to decrease waste materials, etc. (Miranda et al., 2008). In several cases, the search for the aim does not examine the feasibility of processes. This property is understood as the occurrence of the required or desired phenomena. Depending on their physical laws, there are specific conditions on operative variables that guarantee the designed transformation, the expected production or the proper reaction transformation (Almeida-Rivera and Grievink, 2004; Shah et al., 2012). With processes where equilibrium phenomena happen (liquid-vapor equilibrium, forces balance, phases stability, chemical or biological equilibrium), these conditions are more restrictive. For this reason, it is important to characterize correctly the feasibility of processes.

A normal practice to find the best operating point is to search in a wide range of values, expecting that all points inside this range are feasible. But even if this search gives an optimal operating point, it is not guaranteed if expected disturbances on the processes will move the system to a no-feasible state. Cost optimization problems only take into account constraints on operative variables based on safety on operation without examining if those restrictions over or underestimated the whole feasible set of conditions (Grossmann et al., 1983; Heese et al., 2019). When the optimization includes the feasibility of processes in the search, there are strong assumptions over this set to ease its mathematical formulation.

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It is noticed then the necessity to have a methodology to characterize and formulate the feasible sets for any process, that helps to design, control, and optimize the operative condition of them, without losing information, under or overestimation, or strong assumptions over the shape or size of this set. This work is structured as follows: Section 2 presents previous approximations to the feasible set definition and the proposed definition for this work. Section 3 defines the methodology to characterize and get the mathematical formulation for any feasible set. A cost function based on feasibility is also proposed in this section. Section 4 illustrates the proposal on a Reactor-Separator-Recycle system by simulation. Section 5 describes finally the conclusions of this work.

2. BACKGROUND

Although feasibility is a notion of process engineering, there is not a formal definition in literature. However, there are some definitions in other fields that help to conceptualize this term for our aim. Our proposal is based on the definition of feasibility in optimization problems and the reachable set definition in control theory. From the optimization field, we use the concept of the region where mathematical restrictions are satisfied, while from the control theory, the problem is treated considering the input point of view. Those definitions are presented below.

2.1 Feasible set in optimization

In optimization problems, the feasible set is the region on the space of decision variables that satisfies all constraints (Liu et al., 2017; Wright and Nocedal, 1999). A nonlinear program (NLP) is formulated as follows:

$$\begin{aligned} &\min_x \; f_0(x) \\ &\text{s.t. } h(x) = 0, \\ &\quad\;\; g(x) \geq 0, \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^n$ is the vector of decision variables. $f_0(x) : \mathbb{R}^n \to \mathbb{R}$ is the objective function to be minimized, which is in general an economical function based on cost and profits of operation; or a performance function that evaluates if process has the required yield or quality production. $g(x) : \mathbb{R}^n \to \mathbb{R}^p$ and $h(x) : \mathbb{R}^n \to \mathbb{R}^q$ are vector functions constrains. The formulation of the feasible set is as follows (Dinh et al., 2010; Wright and Nocedal, 1999)

$$\Omega = \{x \in \mathbb{R}^n \,|\, h(x) = 0,\, g(x) \geq 0\}. \tag{2}$$

For processes, inequalities define the feasible set, representing safety conditions (to avoid extreme temperatures, pressures, concentration, currents or irradiation) or to fit some required conditions (purity, quality of the final product, demands, etc).

2.2 Reachable set in control theory

For dynamic systems, the reachable set is a region on space state that processes can achieve from a set of the possible initial conditions, and operating with control actions of a set of admissible inputs in an instant. In other words, the reachable set is the space of the dynamic behavior of the process over probable operative conditions. Let us consider a model process defined as follows

$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t), \mathbf{u}(t)) \tag{3}$$

where the $x(t) \in X \subseteq \mathbb{R}^n$ represents the process dynamic state, X the set of state values, $u(t) \in U \subseteq \mathbb{R}^m$ defines the input of process and U the set of available inputs (Alzate Garcés, 2013; Bravo et al., 2005). In this way, the process will develop a specific dynamic behavior depending on the manipulation actions and its current state,.

Let us define the region of state at time t as the set Θ_t. The Reachable Set $R_{t+\tau}(\Theta_t)$ is defined as the region of reached state at the time $t+\tau$, beginning from Θ_t set, applying all control actions within the set U (Zuluaga Bedoya, 2015; Bravo et al., 2005; Bicchi et al., 2002; Gillula et al., 2010), i.e.

$$\begin{aligned} R_{t+\tau}(\Theta_t) = \{x(t+\tau) \in X | \exists x(t) \in X \\ \vee\;\; u \in U : \dot{x}(t) = f(x(t), u(t))\}. \end{aligned} \tag{4}$$

This definition is exemplified on Figure 1. It shows the transition form initial set Θ_t to $R_{t+\tau}(\Theta_t)$ when different action inputs are applied.

The available set of input variables $u(t) \in U$ to find the set $R_{t+\tau}(\Theta_t)$, is generally defined by economical restrictions (range on flow rates, admissible heating depending on available fuel, size of pipes, etc.). Note that this definition is not based on the existence of the phenomena on processes.

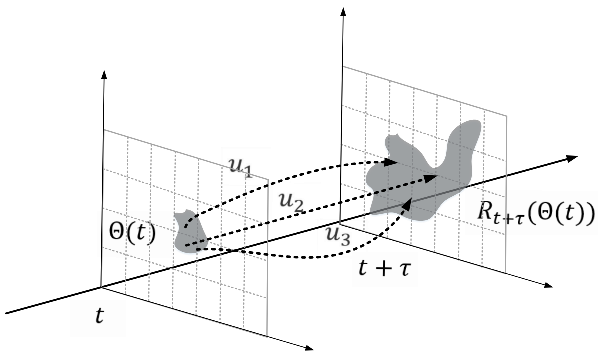

Fig. 1. Reachable set definition from Set control theory.

3. FEASIBLE SET CHARACTERIZATION

As the previous section showed, the feasible set of operative condition for a process is not well defined. This section presents a review of related concepts that will help to understand the proposed definition of the *Feasible Set* index in this work.

3.1 Feasible set definition

Let consider the space of the states and inputs $W \subset \mathbb{R}^n \times \mathbb{R}^m$. Considering $w = [x,\, u]^T$, the feasible set Φ is defined as follows,

$$\Phi = \{w \in W | \Psi(x, u) = 1\}. \tag{5}$$

Different formulations for function $\Psi(x, u)$ can be found in literature, generating different definitions for the feasible set. The formulation could respond to an economic limitation on production, security restrictions or physical capacity of the devices. In this sense, we propose to treat the feasibility through the examination of the inherent phenomena of processes. In this way, $\Psi(x, u)$ determines whether the operative condition guarantees the happening of the required phenomena for the existence of processes. Generally, the equilibrium conditions are defined in this form.

Equilibrium conditions are commonly set by equalities. Let call $g_{\text{eq}}(x, u)$ the mathematical description of equilibrium, depending on input variables u and the state of the process x. In this sense, the formulation for Ψ is as follows

$$\Psi(x, u) = \begin{cases} 1, & \text{if } g_{\text{eq}}(x, u) = 0 \\ 0, & \text{if } g_{\text{eq}}(x, u) \neq 0 \end{cases}. \tag{6}$$

The main difference of this proposal with previous approaches is the use of equilibrium function $g_{\text{eq}}(x, u)$, which is not related to the safe operation, economics limitation or dimensional restrictions. This function comes from physical laws, describing the existence of a particular phenomenon. The function $g_{\text{eq}}(x, u)$ is independent of the dynamic model, which is set by mass and energy balances.

3.2 Characterization of feasible set

As first attempt, it is possible to find a mathematical formulation for the boundary hypersurface of the feasibility set. Normally, this formulation is done with a piecewise functions (Goshtasby, 1986; Schäffer and Van Wyk, 1987) and the belonging of a point on the set is done by checking with a set of inequalities according with the region of validity of each formulation. For low dimension of W, this idea can be implemented, however when the dimension is increased, the complexity to find the mathematical expressions also increases (Bennett and Mangasarian, 1994; Duckham et al., 2008). Due to this complexity, in most cases an under or overestimation with regular hypersurfaces of the original set is applied, which is mathematically possible but not suitable for the real representation of feasible set of processes.

In this way, we propose to use the Medial Axis or Voronoi-skeletons (Xia and Tucker, 2011; Chen and Ma, 2018; Fowler, 2019) in a novel way to characterize the feasible set. We present the steps below.

1- Compute the set Φ using Monte Carlo, or by generation of a grid on W space.
2- Identify the collections of points on the boundary of feasible set, $\partial\Phi$, as the points that are not fully surrounded by other points. These points are denoted by w_b.
3- Compute the Euclidean distance (also known as norm 2) between the point $w_i \in \Phi$ and the j points in the boundary $w_{b_j} \in \partial\Phi$, generating the vector $d_{ij} = \left\|w_i - w_{b_j}\right\|_2$. Then, pick the minimum element of vector d_{ij} (that is the distance to the nearest boundary element). This step is known as the construction of Distance Field Map (DFM), defined as follows

$$DFM(w_i) = \begin{cases} \min(d_{ij}), & \text{if } w_i \in \Phi \\ 0, & \text{if } w_i \notin \Phi \end{cases}. \quad (7)$$

4- Compute the numerical Laplacian $\nabla^2 DFM(w)$.
5- Find the maximum value of Laplacian, $\delta_{\max}$.
6- Select a criteria of acceptance of vertex $0 < \varepsilon < 1$
7- Identify the Medial Axis set by the points $w \in \Phi$ such that $\nabla^2 DFM(w) > \varepsilon\, \delta_{\max}$.
8- Assign to each point of Medial Axis set, $w_{i_{\mathrm{MA}}}$, its distance to boundary $d_{ij_{\mathrm{MA}}}$.

This algorithm starts by generating a collection of points of set Φ (step **1**) and identifying the ones placed on the boundary (step **2**). Then, for all inner points, it is gotten the DFM by computing for each inner point, the distance to all boundary elements, and assigned the lowest value (step **3**). Subsequently, the algorithm identifies the points with the maximum DFM value. To this aim, Laplacian operator is used (Xia and Tucker, 2011) (step **4**). Then, the maximum value of Laplacian is found (step **5**), and a criteria of acceptance ε is selected (step **6**). They characterize the points whose Laplacian fit the criteria (step **7**), identifying finally the inner points $w_{i_{\mathrm{MA}}}$ that are placed on the Medial Axis (step **8**).

Another way to understand the previous algorithm is to find the collection of the center of the biggest inscribed hypersphere. Figure 2 represents an example of Medial axis on a 2D set, as the collection of centers of the largest inscribed circles (skeleton). Note that regardless of the dimension of W space, Medial Axis summaries well the shape and size of the feasible set. Beside, feasibility set depends only on equilibrium equations, and it is invariant for a given problem. In this sense, the set can be characterized off-line efficiently through this methodology.

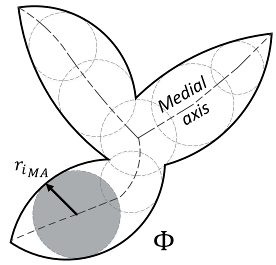

Fig. 2. Medial axis example on Φ set

3.3 Feasibility index

A collection of hyperspheres characterizes the Medial Axis of the feasible set. This collection includes the center and radius of each hypersphere. With this information, analysis of feasibility can be performed. We propose an index that quantifies the feasibility of any input operative condition, instead of using the traditional binary function of belonging *yes/no* index. The objective is to rank better the points on the Medial Axis, because when processes operate in this condition, it is less probable that disturbances will carry the process out of the feasible set. In other words, points near to the boundary have the worst rank. We propose the following feasibility index, $Ind_\Phi(u)$,

$$Ind_\Phi(u) = \frac{1}{N}\sum_{i=1}^{I} \exp\left[-5\left(\frac{\left\|u - u_{i_{\mathrm{MA}}}\right\|_2}{r_{i_{\mathrm{MA}}}}\right)^2\right], \quad (8)$$

where the distance of the operative condition u with the I elements of centers $u_{i_{\mathrm{MA}}}$ on the Medial Axis set is computed and compared with the largest radius of the hypersphere $r_{i_{\mathrm{MA}}}$. N is the number of hyperspheres that intercept the operative condition u. The bell functions $\exp[-(x^2)]$ allow to evaluate this ratio, and all evaluations are summed. It is important to highlight that factor 5 in the exponential function guarantees that points in the bounder of each hypersphere ranked with zero feasibility. The computation of the proposed feasibility index is sightly affected by the dimension of the vector u, because the computation of the Euclidean distance (norm 2) is the only vector operation for which efficient algorithms are available. Once this norm is found, the index works only with scalar quantities.

For a 2D case, Figure 3 represents the evaluation of feasibility index, $Ind_\Phi(u)$, for a set that is characterize by three circles.

This index can be used for different tasks, as simultaneous control and design of processes, Model predictive control (MPC) formulation, or operative points determination. In this way, the feasibility can be quantified, finding the best condition in each case. In this paper, we propose to use the feasibility index to determine the set point of controllers, formulating an optimization problem defined by Eqs. (9). The problem will find the set-point, y_{ref}, subject to the dynamic behavior of the model of processes, Eq. (9b),

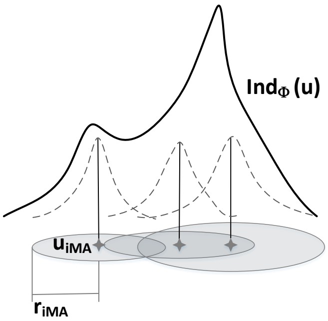

Fig. 3. Feasibility index scheme for a 2D case.

under probable disturbances d, the available measures y, Eq. (9c), the error e, Eq. (9d), the PID law control, Eq. (9e), and restriction on manipulated variable, Eq. (9f), on the time of simulation defined by the interval (9g).

$$\min_{y_{ref}} \quad -\|Ind_\Psi\| \tag{9a}$$
$$\text{subject to} \quad \frac{dx}{dt} = f(t,x,u,d) \tag{9b}$$
$$y = g(x,u) \tag{9c}$$
$$e = y_{ref} - y \tag{9d}$$
$$u = K_P e + K_I \int_0^{t_f} e\,dt + K_D \frac{de}{dt} \tag{9e}$$
$$u_{min} \leq u \leq u_{max} \tag{9f}$$
$$0 \leq t \leq t_f \tag{9g}$$

Note that the objective function of the optimization problem, Eq (9a), is formulated with the feasibility index.

4. CASE OF APPLICATION

We prose to evaluate the presented methodology using a reactor-separator-recycle (RSR) model. The dynamic model is presented in (Morales R. and Alvarez, 2019). This model considers the level and concentration dynamics in the reactor, pressure and concentration dynamics on vapor-phase in the flash tank and level and concentration dynamics on liquid-phase in the flash tank. This process treats a binary mix of components A and B, following the reaction $A \rightarrow B$, supposing the product is more volatile than the reactant, and the component equilibrium follows the Herny's law for constant of separation. The Figure 4 shows the process diagram.

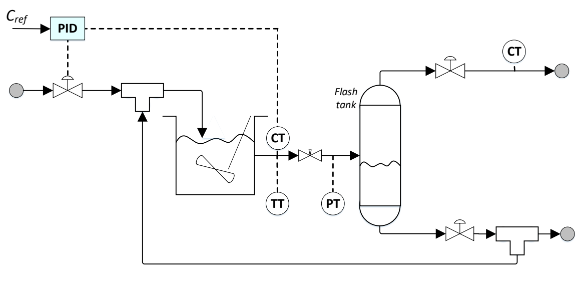

Fig. 4. Reactor-Separator-Recycle process with feedback control loops.

The feasibility of this process is determining if an adiabatic separation is done. The temperature and concentration in the reactor's outlet flow and pressure on the flash tank must follow the Rachford & Rice phase-equilibrium model (Okuno et al., 2010). A closed-loop system controls the reactor's outlet flow concentration. The set-point must guarantee the process inside the feasible set beside the variations on disturbances. In that sense, we propose to find the reference value for the controller to guaranty the feasibility through the feasibility index and improving productivity. The method is explained below.

4.1 Feasibility set characterization

Rachford & Rice phase-equilibrium model $g_{\text{R\&R}}(z,T,P)$ compute the liquid fraction in the separation, which is equal to 0 if all mix reach the vapor state; or 1 if the liquid state is achieved. In this case the function $\Psi(z,T,P)$ is defined as follows

$$\Psi(z,T,P) = \begin{cases} 1, & \text{if } 0 < g_{\text{R\&R}}(z,T,P) < 1 \\ 0, & \text{otherwise} \end{cases}. \tag{10}$$

A grid of size $50 \times 50 \times 50$ (125000 point) on operative variables (z,T,P) was employed to evaluate $\Psi(z,T,P)$. Thus, the feasible set Φ is sketched in Figure 5 with the feasible points (10669 points).

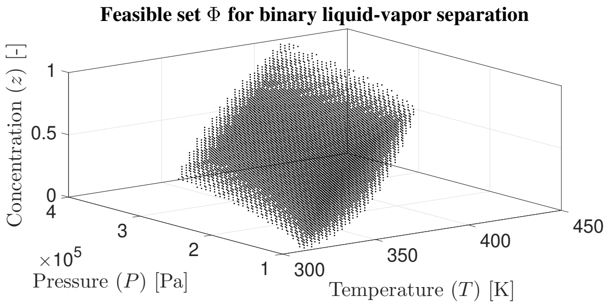

Fig. 5. Feasible set for liquid-vapor equilibrium.

After performing the proposed characterization methodology, the Medial Axis set for the 3D space is found, as shown in Figure 6. This figure has a set of 886 points. It is important to highlight that each point represents the center of a sphere. Each point is associated with its respective radius, which allows the representation of the original feasibility set. The Medial Axis set to describe the whole 3D set has only 8.3% (886/10669) of the initial feasible set points, representing its shape and size.

4.2 Determining optimal operation point

The objective in this process is to find an operative point to get the maximum quantity of the product and that is placed inner of the feasible set. In this sense, we propose to work with the feasible index describe by Eq. (8), and the production rate index defined as follows.

$$Ind_p(u) = \frac{\dot{m}_v C_2}{\rho_v}, \tag{11}$$

where $\dot{m}_v$ is the mass flow in vapor phase out of flash tank, C_2 the concentration of product in vapor phase and ρ_v

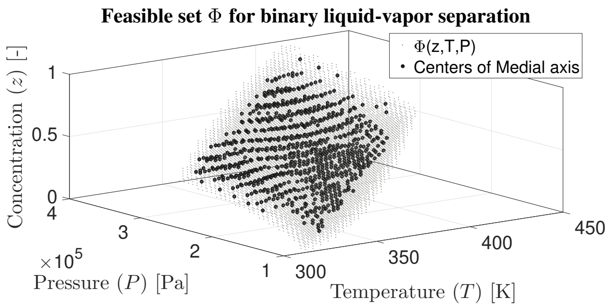

Fig. 6. Collection of centers on the Medial axis.

the density of the vapor. The global objective function is a lineal combination of production rate index and feasible index $Ind_p(u) + Ind_\Phi(u)$.

Next, we formulate the optimization problem defined by Eqs. (9), but modifying the objective function including the productivity index, Eq. (11). After solve this problem, it is determined as optimal set point the concentration equal to 0.586.

4.3 Analysis of results

It is compared, by simulation, the nominal set point of the process $y_{ref-NOM} = 0.63$ given by the steady-state of the plant, and the optimized operative point $y_{ref-OPT} = 0.586$. Both cases are simulated under the same step changes in the input concentration of the reactant and the temperature reactant. Those changes are presented in Figure 7. Also, the process starts at a different point from the steady-state to simulate the plant startup.

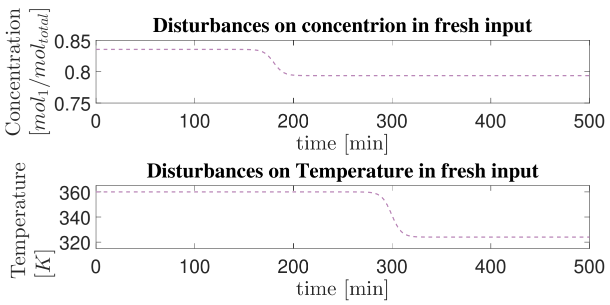

Fig. 7. Disturbances on concentration of reactant and temperature in fresh feed flow.

The controlled variable is shown in Figure 8 for both cases. It is important to highlight that at the end of simulation, the process that follows the nominal reference reaches the instability.

Figure 9 shows the behavior of the Ind_Φ under disturbances. In the nominal case $y_{ref-NOM}$, the index is almost lower than the optimal case $y_{ref-OPT}$. That means in the nominal case, the disturbances carry the process near to the boundaries of the feasible set. In the optimal case, the process can deal even with stronger disturbances. Also, we highlight that the feasibility index reaches the zero value for the nominal case. This explains the instability of the process at the end of the simulation.

Finally, Figure 10 compares the behavior of the productivity rate. It is shown that the nominal operation $y_{ref-NOM}$ has a less production rate than optimal case $y_{ref-OPT}$ out of the flash tank. It is noticed too that when the nominal case becomes unstable, its production rate goes to zero. The reason for this result is because the process went out of the feasible set, and the state (T, P, z) at the end does not allow the liquid-vapor equilibrium. In this sense, there is not a vapor phase.

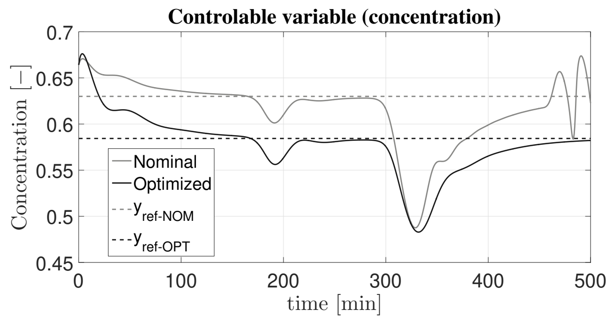

Fig. 8. Dynamic behavior of concentration out of thank reactor.

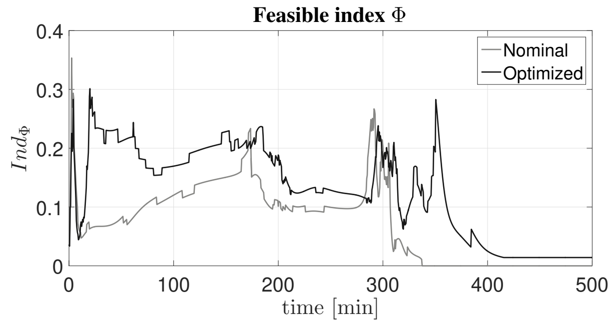

Fig. 9. Behavior of Ind_Φ under disturbances

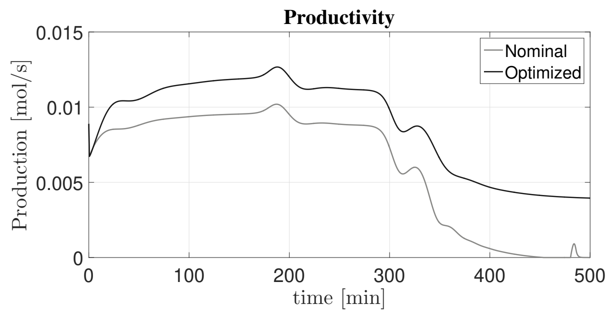

Fig. 10. Behavior of rate of production Ind_p under disturbances

The Table 1 summarizes the previous. It is shown that feasible index was increased as the production index.

Table 1. Margin settings

	Ind_Ψ	Ind_p	$Total$
Nominal	3.0860	0.22916	3.3152
Optimal	4.7246	0.29816	5.0227

A third set-point was found, by only optimizing the productivity index. However, simulation of the process under the describe disturbances in Figure 7 was not possible, because the process goes out of the feasible set and the dynamic simulation does not have a solution. This result shows the necessity to use a procedure to measure the feasibility index instead of a belonging function. In this result, the optimized point by only economical goal is placed near to the boundary, and disturbances are strong enough to shift the states out of the set.

5. CONCLUSIONS

In this work a formal definition for the feasible set of processes based on the physical laws that describe its behavior is presented. In general, these laws are based on equilibrium formulated by algebraic equations and related to the states and input variables on processes. It is important to highlight that the feasible region is not associated with the dynamic model of the process. The model describes the evolution of the states, that must fit on restrictions of the feasible set.

Further, an algorithm to characterize the feasible set was explained, based on the Medial Axis methodology. This algorithm allows us to represent efficiently a set of points without assumptions in its shape or surface. In this way, it is guaranteed that not under or overestimation will be done. The synthesis of the set by the Medial Axis is an arrangement of the centers and radius of maximum inscribed hyperspheres inside the set. With this formulation, the belonging of a point is done by measuring if any distance from the point to centers is less than their respective radius. Working with this vectorial characterization rather than the original algebraic constraints makes it easiest to treat the belonging problem. Based on the previous formulation, a feasibility index was proposed. It makes it possible to quantify the belonging of a point, based on how far to the boundary of the set is placed. In this way, it is changing the usual determination by binary yes/no belonging function.

Finally, the proposed methodology was applied in a Reactor-Separator-Recycle process by simulation. The proposal allows the determination of the set-point that will assure that disturbances will not carry the process out of the feasible set. Through this example is demonstrated that the proposed methodology can be couple with different control tasks. It can be used to determine online the set point according to the presented disturbances, or even to tune the PID controllers when a new set-point is found.

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