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**Evaluation and Redesign for Improving Flexibility In Linear
Systems with Infeasible Nominal Conditions**

by

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**EVALUATION AND REDESIGN
FOR IMPROVING FLEXIBILITY IN LINEAR SYSTEMS
WITH INFEASIBLE NOMINAL CONDITIONS**

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ABSTRACT

This note deals with the problem of evaluating the flexibility index for existing designs for which the new nominal value of operation of the uncertain parameters is infeasible. In this case one can not inscribe within the region of operation the largest hyperrectangle to determine the flexibility index. However, it is shown that for linear systems a negative value of the index can be defined in terms of active sets of constraints that limit flexibility. Furthermore, it is shown that the optimal redesign to increase flexibility can easily be obtained with the procedure by Pistikopoulos and Grossmann (1987). A small example is presented to illustrate these ideas.

INTRODUCTION

Current methods for the evaluation of the flexibility index for a given design assume that the nominal point 0^N of the uncertain parameters is feasible for the operation of a given process (see Swaney and Grossmann, 1985). The same assumption holds for the definition of the resilience index for the heat exchanger networks, by Saboo and Morari (1986). This assumption, however, is only generally true for a *grassroot* design where feasible designs are selected for the nominal parameter values. In the redesign of a process, however, it is very often the case that new desired conditions of operation might result in a situation where the nominal point d^u is infeasible.

Two basic questions that then arise for such a case are the following:

- (i) How to define and compute the flexibility index F for an existing design whose nominal parameter point is infeasible?
- (ii) How to incorporate the infeasible nominal point within a redesign procedure for improving process flexibility?

It is the purpose of this note to show that for linear process models question (i) can be handled by the application of an active set strategy for flexibility analysis, and that question (ii) can be answered by a straightforward extension of the procedure described in Pistikopoulos and Grossmann (1987) for improving flexibility in the retrofit of linear systems.

FLEXIBILITY INDEX FOR INFEASIBLE NOMINAL POINT

In order to illustrate the problem of defining flexibility for a design with infeasible nominal point, consider that the specifications of a design are given by the following four linear inequalities:

$$f_1 = z - d_y \cdot 0_2/2 + d_1 - 3d_2 \leq 0$$

$$f_2 = -2 - dp - 6_2 + d_2 \cdot 1/3 \leq 0$$

$$f_3 = z + \theta_1 - \theta_2 - d_1 - d_2 \leq 0 \quad (1)$$

$$f_4 = z + 13/21 \theta_1 + 5/3 \theta_2 - d_1 - d_2/3 \leq 0$$

The above inequalities involve one control variable z , two design variables d_1 and d_2 and two uncertain parameters θ_1 and θ_2 . It will be assumed that the existing design has values of the design variables of $d_1^E=7$, $d_2^E=4$, and that the nominal point for the uncertain parameters has the values of $\theta_1^N=8$, $\theta_2^N=5$. Expected parameter deviations along the positive and negative directions are also specified as follows: $\Delta\theta_1^+ = \Delta\theta_2^+ = 2$, $\Delta\theta_1^- = 4$, $\Delta\theta_2^- = 3$.

For a given design d , the parametric region of feasible operation, R , is defined by those θ -points for which the feasibility function $f(d, \theta) < 0$ (see Swaney and Grossmann, 1985). The function $f(d, \theta)$ is given by the minimization of the maximum constraint value; that is, $f(d, \theta) = \min_{z, \theta} \max_j \{f_j(d, z, \theta)\}$. The corresponding Kuhn-Tucker conditions of $f(d, \theta)$ as applied to (1) yield:

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 &= i \\ x_1 - x_2 + x_3 + x_4 &= 0 \\ x_1, x_2, x_3, x_4 &\geq 0 \end{aligned} \quad (2)$$

Since there is one control variable z , there are three sets of two active constraints that can potentially limit flexibility (Grossmann and Floudas, 1987). In particular, the constraints that can satisfy (2) are: f_1, f_2 , f_1, f_3 , f_2, f_3 . $J^2 = \{f_v^f, J^2\}$ with $X_1 > X_2 > 0.5$, $J^2 = \{f_1, f_2, f_3\}$ with $X_1^2 = X_2 = 0.5$. Also, since for the k 'th active set $f^k(d, \theta) = z + X_1^k f_1(d, z, \theta)$ (see Pistikopoulos and Grossmann, 1987) this yields the following feasibility functions for the existing design:

$$\begin{aligned} f^1(d) &= -2/3 \theta_1 - 0.25 \theta_2 - 0.335 \\ f^2(d) &= d_1 - \theta_2 - 1.835 \\ f^3(d) &= d_1 + d_2 - 2 \end{aligned} \quad (3)$$

Figure 1 shows the feasible region R , whose boundary is determined by setting $f^k(d, \theta) = 0$ in (3) for each active set $k=1,2,3$. The rectangle T , which is centered at the

nominal point and with sides equal to the expected deviations, represents the *desired* region of operation with flexibility index $F=1$. That is $T=T(F)=\{0 \mid 0^N - FA0^* \leq 0 \leq 0^N + FA0^+\}$ where $F=1$. To determine the actual flexibility index F in Figure 1, the largest rectangle $T(F)$ that is proportional to T must be inscribed within the region of operation. However, from Figure 1 it is clear that this, is not possible since the nominal point $0^N=[5,5]$ is infeasible. Hence, in this case the flexibility index F cannot be estimated from the general formulation (see Swaney and Grossmann, 1985):

$$F = \max h$$

$$\text{s.t. } \max_{0 \in T(F)} \min_z \max_{\mu_j} f_j(d, z, 0) \wedge 0 \quad (4)$$

$$TU)=\{0 \mid 0^N - 2A19' \leq 0 \leq 0^N + 5A < T\}, \quad 5 > 0$$

In the next section, however, it will be shown that despite the fact that problem (4) can not be solved for infeasible 0^N , a flexibility index F can still be defined in terms of the active sets. The geometric interpretation, however, is different from the one used when the nominal point is feasible.

ACTIVE SETS FOR THE FLEXIBILITY INDEX

An alternative formulation to determining the flexibility index in the case of linear systems, consists of finding the smallest scaled deviation from the nominal point to the boundary of the region for each active set (Grossmann and Floudas, 1987). That is,

$$F = \min_{k=1,2,3} \{ d^k \}$$

$$\text{s.t. } \wedge^k (d \cdot 0^N + S^k A 0^{ck}) = 0 \quad k=1,2,3 \quad (5)$$

where $A 0^{ck}$ is the critical parameter direction. As discussed in Pistikopoulos and Grossmann (1987) the critical directions can be obtained by analyzing the signs of $By^k ldd$, $k=1,2,3$, and expressed in terms of the expected deviations. Hence, from (3) it follows that the critical directions for each active set are given by,

$$A0^0 = [-4, -3], \quad A0^{C12} = [2, -3], \quad A0^{C13} = [2, 2] \quad (6)$$

and these are shown in Figure 1. Based on these critical directions, the values of d^k can be determined from the constraint in (5) by solving the equations $\sum_{k=1}^{n_{AS}} \delta^k A0^{Ck} = 0$. From (3) this then leads to the following results:

$$a^1 = 1.44, \quad a^2 = 1.41, \quad \delta^3 = -0.4 \quad (7)$$

Hence, from (5), the flexibility index F exhibits a *negative* value, $F = -0.4$. The interpretation of this value is that it represents the fractional deviation along the *negative* direction of $A0^{C13}$ and that reaches the boundary $f^2 = 0$ (see point A in Figure 1). The negative value of F is then due to the fact that the inequality $\sum_{k=1}^{n_{AS}} \delta^k A0^{Ck} \leq 0$ is infeasible for the nominal point $\#^N = [5, 5]$. Hence, using the concept of active sets one can still define a flexibility index for infeasible nominal points, although in this case the index takes a negative value.

REDESIGN THROUGH ACTIVE SETS

Pistikopoulos and Grossmann (1987) have proposed the following MILP formulation for determining the cheapest retrofit design modifications to increase the flexibility to a specified flexibility target F^1 :

$$\begin{aligned} & \min_{w, Ad} \quad c^T w + JS^T Ad \\ & \text{s.t.} \quad \delta^k \geq F^1 \end{aligned} \quad \left. \vphantom{\begin{aligned} & \min_{w, Ad} \quad c^T w + JS^T Ad \\ & \text{s.t.} \quad \delta^k \geq F^1 \end{aligned}} \right\} k=1, \dots, n_{AS}$$

$$\delta^k = \delta^k_0 + \sum_{i=1}^r \sigma_i^k \Delta d_i \quad (8)$$

$$- U_i^- w_i \leq \Delta d_i \leq U_i^+ w_i, \quad w_i = 0, 1, \quad i=1, \dots, r$$

$$Ad \in GR^r$$

where Δd_i are the design changes associated with 0-1 variables w_i , $i=1, \dots, r$; U_i^+ , U_i^- are bounds for the design changes; c and JS are cost coefficients for the fixed-charge cost model; δ^k is the flexibility index that is predicted for each of the n_{AS} active AS

sets of constraints given the design changes Δd_i ; δ_o^k is the flexibility index for the k 'th active set at the existing design, and σ_i^k are linear sensitivity coefficients. Note that in problem (5), δ_o^k is not restricted to have positive values, and therefore this formulation can be applied for negative values of δ_o^k as will be shown below.

To apply the formulation in (8) to the example problem, the linear sensitivity coefficients σ_i^k have to be calculated as given by the equation (see Pistikopoulos and Grossmann, 1987):

$$\sigma_i^k = \frac{\partial \delta^k}{\partial d_i} = -v^k \sum_{j \in J_A^k} \lambda_j^k \frac{\partial f_j}{\partial d_i} \quad (9)$$

$$\text{where } v^k = - \left[\sum_{i=1}^n \Delta \theta_i^{c,k} \sum_{j \in J_A^k} \lambda_j^k \frac{\partial f_j}{\partial \theta_i} \right]^{-1}$$

The coefficients δ_o^k , $k=1,2,3$ correspond to the values in (7). Hence, the equations for flexibility for each active set in (8) are given as follows:

(i) active set $J_A^1 = \{f_1, f_2\}$: $\sigma_1^1 = 0.2727$, $\sigma_2^1 = -0.5455$, $\delta_o^1 = 1.44$, which leads to

$$\delta^1 = 1.44 + 0.2727\Delta d_1 - 0.5455\Delta d_2$$

(ii) active set $J_A^2 = \{f_2, f_3\}$: $\sigma_1^2 = -0.1249$, $\sigma_2^2 = 0.375$, $\delta_o^2 = 1.41$, which leads to

$$\delta^2 = 1.41 - 0.1249\Delta d_1 + 0.375\Delta d_2$$

(iii) active set $J_A^3 = \{f_2, f_4\}$: $\sigma_1^3 = 0.5222$, $\sigma_2^3 = -0.3501$, $\delta_o^3 = -0.4$, which leads to

$$\delta^3 = -0.4 + 0.5222\Delta d_1 - 0.3501\Delta d_2$$

Assuming cost coefficients $c=(0,0)$, $\beta=(10,10)$ and no bounds for the changes in the design, the MILP in (8) reduces to the LP problem:

$$\min_{\Delta d_1, \Delta d_2} 10\Delta d_1 + 10\Delta d_2$$

$$\text{s.t. } \delta^k \geq F^t \quad k=1,2,3$$

$$\begin{aligned}
 d^1 &= 1.44 + 0.2727Ad_1 - 0.5455Ad_2 \\
 d^2 &= 1.41 - 0.1249Ad_1 + 0.375Ad_2 \\
 d^3 &= -0.4 + 0.5222Ad_1 - 0.3501Ad_2
 \end{aligned}
 \tag{10}$$

Setting the flexibility target equal to one, i.e. $F=1.0$, the above problem (10) yields: $[Ad_1 = 2.682, Ad_2 = 0.0]$ and thus the new design is given by $d_1^{NEW} = 9.682$, $d_2^{NEW} = 4.0$.

The parametric region of this optimal redesign is shown in Figure 2, where the corresponding functions $j^k(d^{NEW}, 0)$ with the new design variables are given by:

$$\begin{aligned}
 j^1(d^{NEW}, 0) &= 23.0 - 0.4 + 1006 \\
 j^2(d^{NEW}, 0) &= 0/3 - 67 - 3.176 \\
 j^3(d^{NEW}, 0) &= 0/7 * B_2/2 - 3.341
 \end{aligned}
 \tag{11}$$

As can be seen in Figure 2 the rectangle T which corresponds to the flexibility index value of $F=1$ is now inscribed within the region of operation of the new design.

CONCLUSIONS

It has been shown in this note that for linear systems, the flexibility index F can be obtained for the case of an infeasible nominal parameter point d^H through the active sets of constraints that may limit flexibility. As was shown, in this case the flexibility index takes a negative value, and represents the fractional deviation along the negative critical direction of the limiting set of active constraints. Furthermore, it has been shown that the procedure described in Pistikopoulos and Grossmann (1987) can handle with no difficulty the case of retrofitting linear designs with infeasible nominal point d^H in order to achieve a desired degree of flexibility.

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REFERENCES

1. Grossmann, I. E. and C. A. Floudas, "Active constraint strategy for flexibility analysis in chemical processes," *to appear in Comp. Chem. Eng.*, 1987.
2. Pistikopoulos, E. N. and I. E. Grossmann, "Optimal retrofit design for improving process flexibility in linear systems/' *accepted for publication in Comp. Chem. Eng.*, 1987.
3. Saboo, A. K., M. Morari and D. C. Woodcock, "Design of resilient processing plants-VIII. A resilience index for heat exchanger networks," *Chem. Eng. Sci.*, Vol. 40, No. 8, p. 1553, 1985.
4. Swaney, R. E. and I. E. Grossmann, "An index for operational flexibility in chemical process design. Part I : Formulation and theory.," *A.I.Ch.E. J.*, Vol. 31, p. 621, 1985.

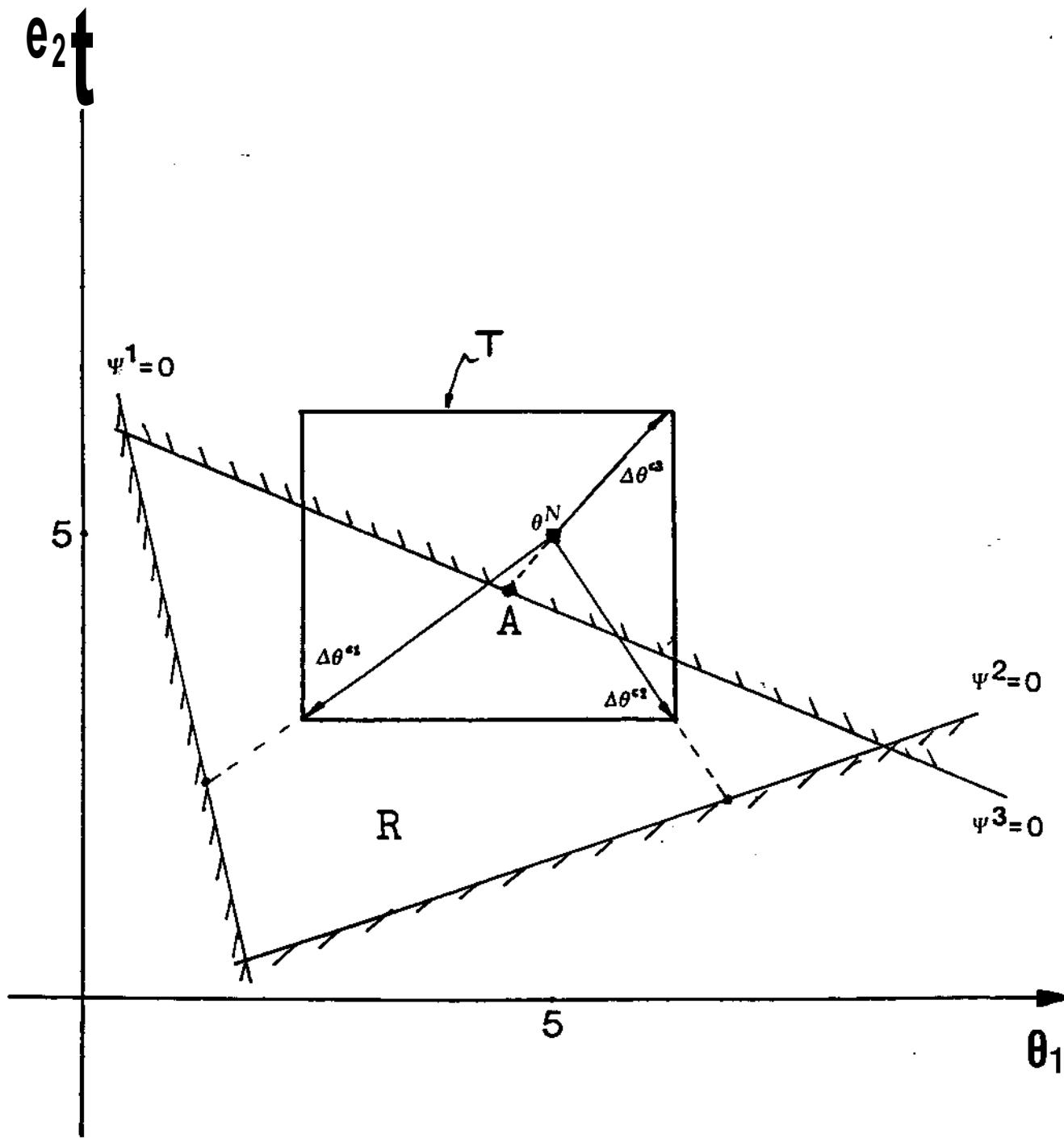


Figure 1: Feasible region of the existing design

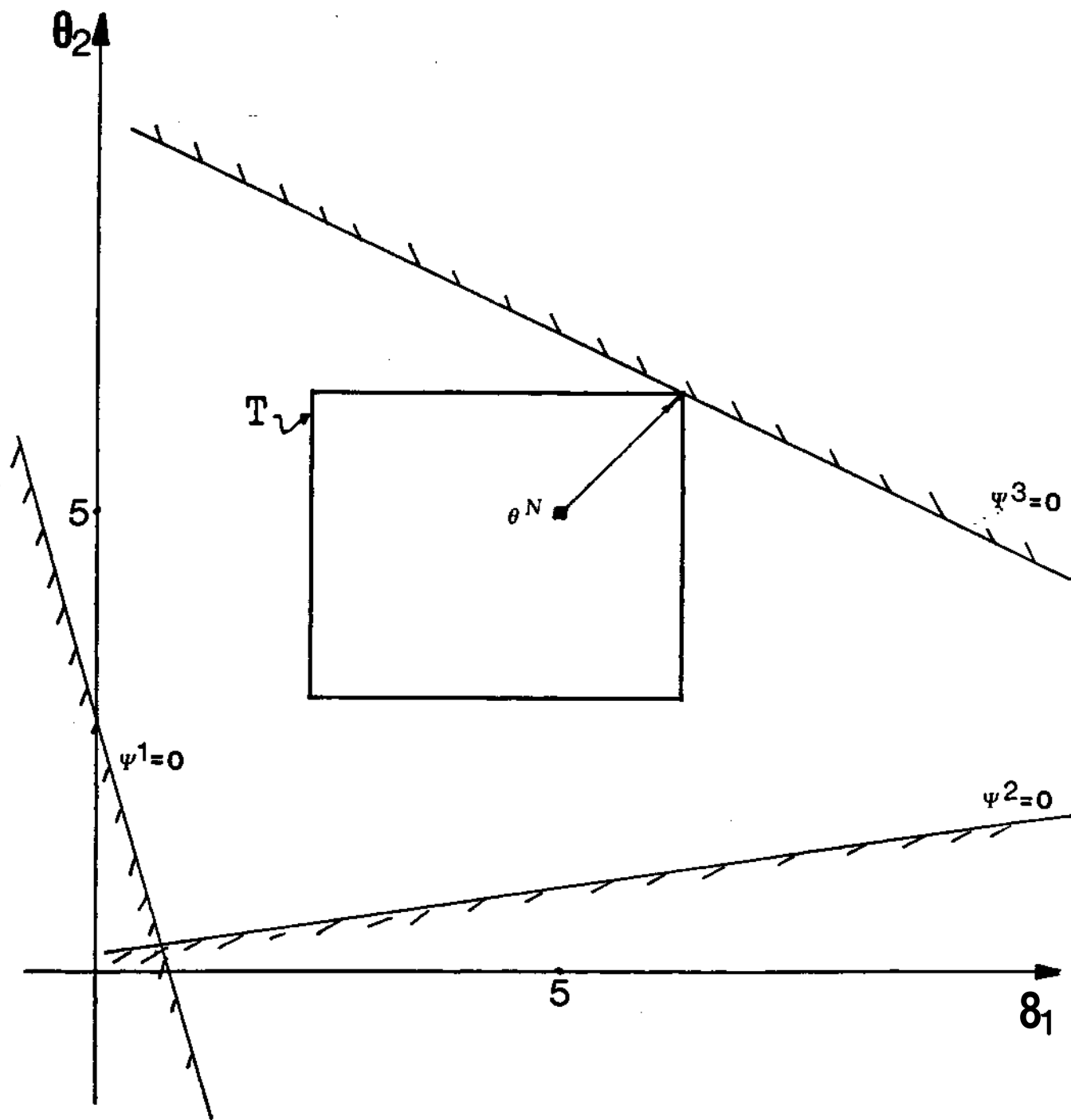


Figure 2: Feasible region of the redesign