

# Optimal Bifunctional Catalyst Problem

SADCO Young Researchers Workshop

Daniel Hoehener

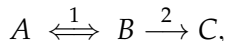
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Based on a paper by R. Jaczson

# THE CHEMICAL ENGINEERING PROBLEM

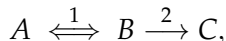
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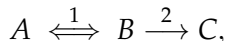


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**Control:** We control the distribution of catalysts 1 and 2 at each point along the reactor. Thus,  $t$  being the position in the reactor,

$$u(t) = \frac{\text{amount of catalyst 1}}{\text{amount of catalyst 1} + \text{amount of catalyst 2}}.$$

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**State Constraints:**  $0 \leq x_i(t) \leq 1, 0 \leq x_1(t) + x_2(t) \leq 1$  for  $i \in \{1, 2\}$  and  $t \in [0, T]$   $\dashrightarrow$   $h(x(t)) \leq 0$ .

## Remark.

The mole fraction of C is  $1 - x_1 - x_2$ .

$k_i$  are rates of reaction.

# PROBLEM FORMULATION

$$\text{Minimize} \quad g(x(0), x(T)) \quad (P)$$

over  $x \in W^{1,1}([0, T]; \mathbb{R}^2)$  and  $u \in \mathcal{M}([0, T]; \mathbb{R})$  satisfying

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Then, since terminal constraints are absent, the maximum principle is normal, i.e.  $\lambda = 1$ .

# PONTRYAGIN'S MAXIMUM PRINCIPLE

The **Hamiltonian** is,

$$\mathcal{H}(x, p, u) = \langle p, f(x, u) \rangle = u [(p_2 - p_1)(k_1 x_1 - k_2 x_2) + p_2 k_3 x_2] - p_2 k_3 x_2.$$



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IMPLIES

$$\bar{u}(t) = \arg \max_{u \in U} \left\{ -k_3 p_2(t) \bar{x}_2(t) + u \underbrace{[(p_2(t) - p_1(t))(k_1 \bar{x}_1(t) - k_2 \bar{x}_2(t)) + k_3 p_2(t) \bar{x}_2(t)]}_{=: J(t)} \right\}.$$

# ANALYTICAL SOLUTION I

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Consequently,

$$J(t) < 0 \longrightarrow \bar{u}(t) = 0$$

$$J(t) > 0 \longrightarrow \bar{u}(t) = 1$$

$$J(t) = 0 \longrightarrow \text{singular case}$$

$$2. p(T) = (-1, -1)$$

IMPLIES

$$J(T) = -k_3 \bar{x}_2(T) < 0 \quad \longrightarrow \quad \bar{u}(T) = 0$$

$$\mathcal{H}(\bar{x}(T), p(T), \bar{u}(T)) = k_3 \bar{x}_2(T) > 0$$

## Structure of the end of optimal trajectories

$J(\cdot)$  decreases as  $t \rightarrow T$  and  $\bar{u} \equiv 0$

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## Interpretation

After some time  $t_0$ , the reaction  $A \rightleftharpoons B$  is stopped.

## CONDITIONS WITH SINGULAR SEGMENT

Going **backwards in time**,  $J(\cdot)$  increases until it reaches 0 at some time  $t_0$ . Then enters either a singular segment or switches to  $\bar{u} \equiv 1$ . Further, as soon as one switches to  $\bar{u}(t) = 1$ , it can be shown that  $J(\cdot)$  will never become 0 again.

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Using this and **computations**, we find that,

$$\bar{u}(t) = \frac{\alpha(1 + \alpha)}{\beta + (1 + \alpha)^2},$$

where  $\alpha := \sqrt{\frac{k_3}{k_2}}$  and  $\beta := \frac{k_1}{k_2}$ .

Obrigado!