Optimal Bifunctional Catalyst Problem

SADCO Young Researchers Workshop

Daniel Hoehener

Institut de Mathématiques de Jussieu
Université Pierre et Marie Curie, Paris, France

Funchal, January 21-23, 2013

Based on a paper by R. Jaczson

Setting: The following chemical reaction takes place in a tubular reactor,

$$A \stackrel{1}{\Longleftrightarrow} B \stackrel{2}{\longrightarrow} C,$$

where the first reaction is reversible and the second is irreversible. The ratio of substances A, B and C evolves according to the current ratios and the ratio between the catalysts 1 and 2.

The Chemical Engineering Problem

Setting: The following chemical reaction takes place in a tubular reactor,

$$A \overset{1}{\Longleftrightarrow} B \overset{2}{\longrightarrow} C,$$

where the first reaction is reversible and the second is irreversible. The ratio of substances A, B and C evolves according to the current ratios and the ratio between the catalysts 1 and 2.

Goal: Maximize the yield of substance C at exit, when pure substance A is fed into the reactor.

The Chemical Engineering Problem

Setting: The following chemical reaction takes place in a tubular reactor,

$$A \overset{1}{\Longleftrightarrow} B \overset{2}{\longrightarrow} C,$$

where the first reaction is reversible and the second is irreversible. The ratio of substances A, B and C evolves according to the current ratios and the ratio between the catalysts 1 and 2.

Goal: Maximize the yield of substance C at exit, when pure substance A is fed into the reactor.

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

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

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0, 1]$ a.e. in $[0, T]$;

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0, 1]$ a.e. in $[0, T]$;

State variables: $x(t) = (x_1(t), x_2(t))$ = mole fraction of A and B;

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0, 1]$ a.e. in $[0, T]$;

State variables: $x(t) = (x_1(t), x_2(t))$ = mole fraction of A and B;

Dynamics: $f(x, u) = \begin{pmatrix} f_1(x, u) \\ f_2(x, u) \end{pmatrix} = \begin{pmatrix} u(k_2 x_2 - k_1 x_1) \\ u(k_1 x_1 - k_2 x_2) - (1 - u) k_3 x_2 \end{pmatrix}$;

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0, 1]$ a.e. in $[0, T]$;

State variables: $x(t) = (x_1(t), x_2(t))$ = mole fraction of A and B;

Dynamics: $f(x, u) = \begin{pmatrix} f_1(x, u) \\ f_2(x, u) \end{pmatrix} = \begin{pmatrix} u(k_2 x_2 - k_1 x_1) \\ u(k_1 x_1 - k_2 x_2) - (1 - u) k_3 x_2 \end{pmatrix}$;

Cost: $g(x^0, x^T) = -1 + x_1^T + x_2^T$;

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0,1]$ a.e. in $[0,T]$;

State variables: $x(t) = (x_1(t), x_2(t))$ = mole fraction of A and B;

Dynamics: $f(x,u) = \begin{pmatrix} f_1(x,u) \\ f_2(x,u) \end{pmatrix} = \begin{pmatrix} u(k_2 x_2 - k_1 x_1) \\ u(k_1 x_1 - k_2 x_2) - (1-u) k_3 x_2 \end{pmatrix}$;

Cost: $g(x^0, x^T) = -1 + x_1^T + x_2^T$;

Endpoint Constraints: $(x(0), x(T)) \in E := \{(1,0)\} \times \mathbb{R}^2$;

Mathematical Model

Let $k_1, k_2, k_3 > 0$. $T > 0$ is the length of the reactor.

Control Constraints: $u(t) \in U := [0, 1]$ a.e. in $[0, T]$;

State variables: $x(t) = (x_1(t), x_2(t))$ = mole fraction of A and B;

Dynamics: $f(x, u) = \begin{pmatrix} f_1(x, u) \\ f_2(x, u) \end{pmatrix} = \begin{pmatrix} u(k_2x_2 - k_1x_1) \\ u(k_1x_1 - k_2x_2) - (1 - u)k_3x_2 \end{pmatrix}$;

Cost: $g(x^0, x^T) = -1 + x_1^T + x_2^T$;

Endpoint Constraints: $(x(0), x(T)) \in E := \{(1, 0)\} \times \mathbb{R}^2$;

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

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

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

$$\begin{cases} \dot{x}(t) = f(t, x(t), u(t)) \quad u(t) \in U \qquad a.e. \\ (x(0), x(T)) \in E \\ h(x(t)) \leq 0 \quad \forall t \in [0,T] \end{cases}$$

Problem formulation

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

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

$$\begin{cases} \dot{x}(t) = f(t, x(t), u(t)) \quad u(t) \in U \qquad a.e. \\ (x(0), x(T)) \in E \\ h(x(t)) \leq 0 \quad \forall t \in [0,T] \end{cases}$$

Note

Hypotheses of PMP are satisfied.

Problem formulation

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

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

$$\begin{cases} \dot{x}(t) = f(t, x(t), u(t)) \quad u(t) \in U \qquad a.e. \\ (x(0), x(T)) \in E \\ h(x(t)) \leq 0 \quad \forall t \in [0,T] \end{cases}$$

Note

Hypotheses of PMP are satisfied.
Assume there exists an optimal solution in the interior of state constaints. Thus we omit them.

Problem formulation

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

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

$$\begin{cases} \dot{x}(t) = f(t, x(t), u(t)) \quad u(t) \in U \qquad a.e. \\ (x(0), x(T)) \in E \end{cases}$$

Note

Hypotheses of PMP are satisfied.
Assume there exists an optimal solution in the interior of state constaints. Thus we omit them.
Then, since terminal constraints are absent, the maximum principle is normal, i.e. $\lambda = 1$.

Pontryagin's Maximum Principle

The Hamiltonian is,

$$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$$

Pontryagin's Maximum Principle

The Hamiltonian is,

$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$

The PMP says that $(\bar{x},\bar{u})$ is a candidate for a local minimum if there exists $p \in W^{1,1}([0,T];\mathbb{R}^2)$ s.t.

1. $-\dot{p}(t) = \mathcal{H}_x(\bar{x}(t), p(t), \bar{u}(t))$ a.e.

Pontryagin's Maximum Principle

The Hamiltonian is,

$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$

The PMP says that $(\bar{x},\bar{u})$ is a candidate for a local minimum if there exists $p \in W^{1,1}([0,T];\mathbb{R}^2)$ s.t.

1. $-\dot{p}(t) = \mathcal{H}_x(\bar{x}(t), p(t), \bar{u}(t))$ a.e.
2. $(p(0), -p(T)) \in \nabla g(\bar{x}(0), \bar{x}(T)) + N_E(\bar{x}(0), \bar{x}(T))$

Pontryagin's Maximum Principle

The Hamiltonian is,

$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$

The PMP says that $(\bar{x},\bar{u})$ is a candidate for a local minimum if there exists $p \in W^{1,1}([0,T];\mathbb{R}^2)$ s.t.

1. $-\dot{p}(t) = \mathcal{H}_x(\bar{x}(t), p(t), \bar{u}(t))$ a.e.
2. $(p(0), -p(T)) \in \nabla g(\bar{x}(0), \bar{x}(T)) + N_E(\bar{x}(0), \bar{x}(T))$
3. $\mathcal{H}(\bar{x}(t), p(t), \bar{u}(t)) = \max_{u\in U} \mathcal{H}(\bar{x}(t), p(t), u)$ a.e.

Pontryagin's Maximum Principle

The Hamiltonian is,

$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$

The PMP says that $(\bar{x}, \bar{u})$ is a candidate for a local minimum if there exists $p \in W^{1,1}([0,T];\mathbb{R}^2)$ s.t.

1. $-\dot{p}(t) = \mathcal{H}_x(\bar{x}(t), p(t), \bar{u}(t))$ a.e.
2. $(p(0), -p(T)) \in \nabla g(\bar{x}(0), \bar{x}(T)) + N_E(\bar{x}(0), \bar{x}(T))$
3. $\mathcal{H}(\bar{x}(t), p(t), \bar{u}(t)) = \max_{u \in U} \mathcal{H}(\bar{x}(t), p(t), u)$ a.e.

$$2. \implies p_1(T) = p_2(T) = -1.$$

The Hamiltonian is,

$\mathcal{H}(x,p,u) = \langle p, f(x,u)\rangle = u\left[(p_2 - p_1)(k_1x_1 - k_2x_2) + p_2k_3x_2\right] - p_2k_3x_2.$

The PMP says that $(\bar{x},\bar{u})$ is a candidate for a local minimum if there exists $p \in W^{1,1}([0,T];\mathbb{R}^2)$ s.t.

1. $-\dot{p}(t) = \mathcal{H}_x(\bar{x}(t), p(t), \bar{u}(t))$ a.e.
2. $p(T) = (-1,-1)$
3. $\mathcal{H}(\bar{x}(t), p(t), \bar{u}(t)) = \max_{u\in U} \mathcal{H}(\bar{x}(t), p(t), u)$ a.e.

Analytical Solution I

3. $\mathcal{H}(\bar{x}(t), p(t), \bar{u}(t)) = \max_{u \in U} \mathcal{H}(\bar{x}(t), p(t), u)$ a.e.

IMPLIES

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

Analytical Solution I

3. $\mathcal{H}(\bar{x}(t), p(t), \bar{u}(t)) = \max_{u \in U} \mathcal{H}(\bar{x}(t), p(t), u)$ a.e.

IMPLIES

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

Consequently,

$$\begin{aligned} J(t) < 0 \quad &\longrightarrow \quad \bar{u}(t) = 0 \\ J(t) > 0 \quad &\longrightarrow \quad \bar{u}(t) = 1 \\ J(t) = 0 \quad &\longrightarrow \quad \text{singular case} \end{aligned}$$

Analytical Solution II

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 $t \to T$ and $\bar{u} \equiv 0$

$\bar{x}_1(\cdot)$ is constant on such a segment

$\bar{x}_2(\cdot)$ decreases

Analytical Solution II

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 $t \to T$ and $\bar{u} \equiv 0$
$\bar{x}_1(\cdot)$ is constant on such a segment
$\bar{x}_2(\cdot)$ decreases

Interpretation

After some time t_0, the reaction $A \iff B$ 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 singlular 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.

Conditions with Singular Segment

Going backwards in time, $J(\cdot)$ increases until it reaches 0 at some time t_0. Then enters either a singlular 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.

Conclusion

The solutions are bang-singular-bang or bang-bang.

Conditions with Singular Segment

Going backwards in time, $J(\cdot)$ increases until it reaches 0 at some time t_0. Then enters either a singlular 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.

Conclusion

The solutions are bang-singular-bang or bang-bang.

On a singular segment we have

$$J \equiv 0 \quad \text{and} \quad \frac{dJ}{dt} = 0.$$

Conditions with Singular Segment

Going backwards in time, $J(\cdot)$ increases until it reaches 0 at some time t_0. Then enters either a singlular 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.

Conclusion

The solutions are bang-singular-bang or bang-bang.

On a singular segment we have

$$J \equiv 0 \quad \text{and} \quad \frac{dJ}{dt} = 0.$$

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 $\beta := \frac{k_1}{k_2}$.

THE END

Obrigado!