MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Periodic Optimal Control of a Plug Flow Reactor Model with an Isoperimetric Constraint

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Content

1. Motivation
2. Plug flow reactor model
3. Plug flow reactor model with two controls
4. Numerical simulations
5. Conclusion and future research

1. **Motivation**
2. Plug flow reactor model
3. Plug flow reactor model with two controls
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5. Conclusion and future research

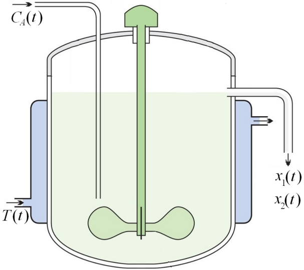
$$V\frac{dC_A}{dt} = F(C_{A_0} - C_A) - kVC_A^n \quad t \in [0,\tau]$$

$$\frac{1}{\tau}\int_0^\tau C_P(t)dt \ \rightarrow \max, \text{ or } \frac{1}{\tau}\int_0^\tau C_A(t)dt \ \rightarrow \min,$$

C_{A_0} is the inlet concentration of A

$$C_{A_0} = \overline{C} = const$$

$$\frac{1}{\tau}\int_0^\tau C_{A_0}(t)dt = \overline{C}$$



C_P is the product concentration

$$C_P = \overline{C}_P = const$$

$$\frac{1}{\tau}\int_0^\tau C_P(t)dt > \overline{C}_P$$

M. Petkovska, A. Seidel-Morgenstern (2012). Evaluation of periodic processes. Chapter 14 in: P.L. Silveston, R.R. Hudgins (Eds.), *Periodic Operation of Chemical Reactors*, 387–413.

Motivation. Continuous Stirred Tank Reactor Model

An isoperimetric optimal control problem with periodic inputs was solved in[1]

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$$\frac{1}{\tau}\int_0^\tau C_A(t)dt \;\to \min,$$

[1] A. Zuyev, A. Seidel-Morgenstern, P. Benner (2017), *Chem. Eng. Sci.*, **161**:206–214.

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$$C_A(0) = C_A(\tau), \qquad \frac{1}{\tau}\int_0^\tau C_{A_0}(t)dt = \overline{C}, \qquad C_{A_0} \in [C_{\min}, C_{\max}]$$

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$$\boldsymbol{C_{A_0}(t) = \begin{cases} C_{\max}, & t \leqslant \tau^*, \\ C_{\min}, & t > \tau^*. \end{cases}}$$

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Motivation. Plug flow reactor model

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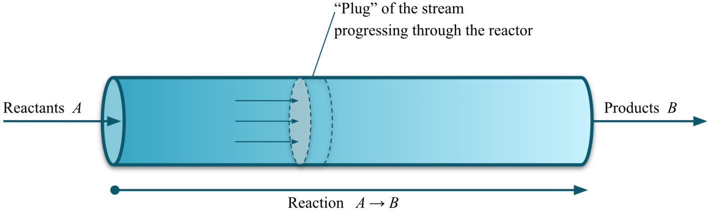

PFR model[2]:

$$\frac{\partial C_A(x,t)}{\partial t} + v\frac{\partial C_A(x,t)}{\partial x} = -kC_A(x,t)^n,\ x \in [0,L]$$

$$C_A(0,t) = C_{A_0}(t) \text{ – control}$$

Cost: $\frac{1}{\tau}\int_0^\tau C_A(L,t)\,v\,dt \ \to \min$

[2]M. Petkovska, A. Seidel-Morgenstern (2013), Evaluation of periodic processes.

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  What is the best (optimal) strategy?

[2] M. Petkovska, A. Seidel-Morgenstern (2013), Evaluation of periodic processes.

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Optimal control problem for PFR model

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Class of admissible controls $\mathcal{U}_\tau$

Let $\tau > 0$, $C_{\max} > C_{\min} > 0$, and $\overline{C} \in [C_{\min}, C_{\max}]$ be given. The class of admissible controls $\mathcal{U}_\tau$ consists of all locally measurable functions $C_{A_0} : \mathbb{R} \to [C_{\min}, C_{\max}]$ such that $C_{A_0}(t)$ is τ-periodic and

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Cost: $\displaystyle \frac{1}{\tau}\int_0^\tau C_A(L,t)\,v\,dt \;\to \min$

Solution and cost functional representation

The boundary value problem is solved by method of characteristics[3]:

$$C_A(x,t) = \left(C_{A_0}\left(t - \frac{x}{v}\right)^{-(n-1)} + \frac{k(n-1)}{v}x\right)^{-\frac{1}{n-1}}, \quad n \neq 1.$$

[3] H. Grabmüller, U. Hoffmann, K. Schädlich (1985)

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The explicit expression of the cost functional:

$$J = \frac{v}{\tau}\int_0^\tau \left(C_{A_0}(t)^{-(n-1)} + \frac{kL(n-1)}{v} \right)^{-\frac{1}{n-1}} dt =: \frac{v}{\tau}\int_0^\tau \Phi(C_{A_0}(t))dt.$$

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The function Φ is concave if $n > 1$ and convex if $n < 1$.

[3]H. Grabmüller, U. Hoffmann, K. Schädlich (1985)

Solution of Optimal Control Problem

Theorem 1[4]

1) If $n = 1$, then $J[C_{A_0}] \equiv J[\overline{C}] \;\; \forall C_{A_0} \in \mathcal{U}_\tau$.
2) If $n < 1$ and $C_{\min} > \left(\frac{v}{kL(1-n)}\right)^{-\frac{1}{1-n}}$, then $\overline{C}$ is optimal.
3) If $n > 1$, then the bang-bang strategy is optimal:

$$C_{A_0}(t) = \begin{cases} C_{\min}, & \text{if } \; t \in A^-, \\ C_{\max}, & \text{if } \; t \in A^+ = [0, \tau) \setminus A^-, \end{cases} \tag{1}$$

and $A^- \subset [0, \tau)$ is any Lebesgue-measurable set such that $\mu(A^-) = \frac{C_{\max} - \overline{C}}{C_{\max} - C_{\min}} \tau$.

[4]Ye.Ye., A. Zuyev, P. Benner, A. Seidel-Morgenstern (2024), JOTA

Sketch of the Proof

Step 1. New class $\mathcal{A}_{\widetilde{C}}$ ($\mathcal{A}_{\widetilde{C}} \subset \mathcal{U}_\tau$)

The function $c : \mathbb{R} \to [C_{\min}, C_{\max}]$ belongs to the class $\mathcal{A}_{\widetilde{C}}$, $\widetilde{C} \in [C_{\min}, C_{\max}]$, if $c(\cdot) \in \mathcal{U}_\tau$ and $\exists\, A^+ \subset [0, \tau)$, $A^- \subset [0, \tau)$ such that:

- $\operatorname{ess\,inf}_{t \in \mathbb{A}^+} c(t) \geqslant \widetilde{C}$, $\operatorname{ess\,sup}_{t \in \mathbb{A}^-} c(t) \leqslant \widetilde{C}$;
- $\mu(A^+ \cap A^-) = 0$, $\mu(A^+ \cup A^-) = \tau$, $\mu(A^-) = \frac{C_{\max} - \overline{C}}{C_{\max} - C_{\min}} \tau$.

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Step 1. New class $\mathcal{A}_{\widetilde{C}}$ ($\mathcal{A}_{\widetilde{C}} \subset \mathcal{U}_\tau$)

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Step 2. Bang-bang strategy is better than any control from $\mathcal{A}_{\widetilde{C}}$:

$$\forall\, C_{\mathcal{A}}(\cdot) \in \mathcal{A}_{\widetilde{C}} \quad \exists\, C_{bang-bang}(\cdot) \in \mathcal{U}_\tau : \quad J[C_{bang-bang}] \leqslant J[C_{\mathcal{A}}],$$

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Step 3. $\mathcal{U}_\tau \subset \mathcal{A}_{\widetilde{C}}$:

$$\forall\, u(\cdot) \in \mathcal{U}_\tau \quad \exists\, \widetilde{C} \in (C_{\min}, C_{\max}) : \quad u(\cdot) \in \mathcal{A}_{\widetilde{C}}$$

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Plug flow reactor model with two controls

$$\frac{\partial C_A(x,t)}{\partial t} + \boldsymbol{v(t)}\frac{\partial C_A(x,t)}{\partial x} + kC_A(x,t)^n = 0, \qquad x \in [0,L],$$
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The class $\mathcal{V}_\tau$ consists of all locally measurable vector-functions $(c, v) : \mathbb{R} \to [C_{\min}, C_{\max}] \times [v_{\min}, v_{\max}]$ such that $(c(t), v(t))$ is τ-periodic and the isoperimetric condition holds:

$$\frac{1}{\tau} \int_0^\tau C_{A_0}(t) v(t) dt = \overline{C}\, \overline{v}$$

Plug flow reactor model with two controls

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$$\frac{1}{\tau}\int_0^\tau C_{A_0}(t)v(t)dt = \overline{C}\,\overline{v}$$

Cost: $J = \dfrac{1}{\tau}\displaystyle\int_0^\tau C_A(L,t)\,v(t)\,dt \;\to \min$

Solution and cost functional representation

The solution is obtained by the method of characteristics ($n \neq 1$):

$$C_A(x,t) = \left[C_{A_0}\left(V^{-1}(V(t)-x)\right)^{-(n-1)} + k(n-1)\left(t - V^{-1}(V(t)-x)\right)\right]^{-\frac{1}{n-1}},$$

where $V(t) := \int_0^t v(\xi)d\xi$ and V^{-1} denotes the inverse to V.

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Consider the additional assumption, that the **residence time** of the reaction is equal to τ, i.e.

$$\int_0^\tau v(t)dt = L \qquad (A1)$$

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Consider the additional assumption, that the **residence time** of the reaction is equal to τ, i.e.

$$\int_0^\tau v(t)dt = L \qquad (A1)$$

The cost functional can be rewritten as follows:

$$J[C_{A_0}, v] = \frac{1}{\tau}\int_0^\tau \left(C_{A_0}(t)^{-(n-1)} + k(n-1)\tau\right)^{-\frac{1}{n-1}} v(t)dt$$

Solution of Optimal control problem

Theorem 2

* If $n = 1$, then $J[C_{A_0}, v] = \overline{C}\,\overline{v}e^{-k\tau} \qquad \forall\,(C_{A_0}, v) \in \mathcal{V}_\tau$.
* If $n > 1$, then bang-bang is the optimal strategy:

$$c(t) = \begin{cases} C_{\max}, & \text{if } t \in A^+, \\ C_{\min}, & \text{if } t \in A^-, \end{cases} \qquad v(t) = \begin{cases} v_{\min}, & \text{if } t \in B^-, \\ v_{\max}, & \text{if } t \in B^+, \end{cases}$$

with the sets

$$A^+, A^- \subset [0,\tau),\ \mu(A^+ \cap A^-) = 0,\ \mu(A^+ \cup A^-) = \tau,$$

$$B^+, B^- \subset [0,\tau),\ \mu(B^+ \cap B^-) = 0,\ \mu(B^+ \cup B^-) = \tau.$$

Their measures are defined by the isoperimetric constraint and *(A1)*. Moreover,

$$\mu(A^+ \cap B^-) \ \to \max\,.$$

Step 1. New class $\mathcal{A}_{\widetilde{C},\,\nu}$ ($\mathcal{A}_{\widetilde{C},\,\nu} \subset \mathcal{V}_\tau$)

The vector-valued function

$$(c, v) : \mathbb{R} \to [C_{\min}, C_{\max}] \times [v_{\min}, v_{\max}]$$

belongs to the class $\mathcal{A}_{\widetilde{C},\,\nu}$, $\widetilde{C} \in [C_{\min}, C_{\max}]$, $\nu \in [0, \tau]$, if $(c, v) \in \mathcal{V}_\tau$ and $\exists\, A^+ \subset [0, \tau)$, $A^- \subset [0, \tau)$ such that:

- $\operatorname{ess\,inf}_{t \in \mathbb{A}^+} c(t) \geqslant \widetilde{C}$,
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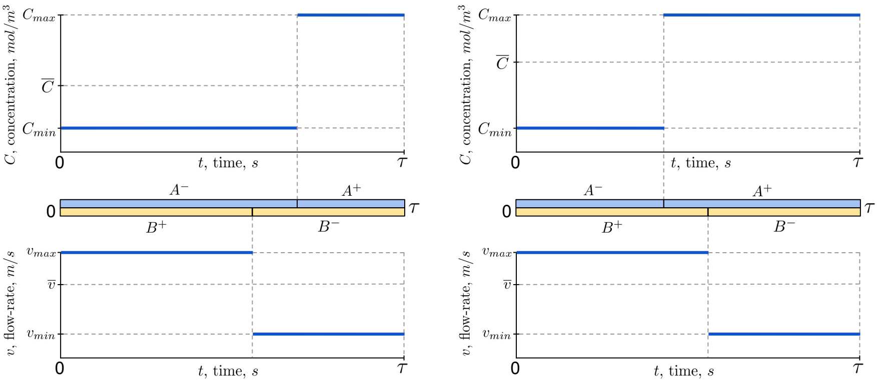
- $\mu(A^+ \cap A^-) = 0$;
- $\mu(A^+ \cup A^-) = \tau$;
- $\mu(A^+) = \nu$.

Step 2. Class $\mathcal{B}_\tau$ with given $\tau > 0$ is a class of control functions $(c, v) \in \mathcal{V}_\tau$ defining the bang-bang strategy with respect to the constraints of the optimal control problem.

Two cases are possible:



Step 3. The bang-bang strategy $\mathcal{B}_\tau$ has better performance than any control from the class $\mathcal{A}_{\widetilde{C},\,\mu(A^+)}$:

$$J[\mathcal{B}_\tau] \leqslant J[\mathcal{A}_{\widetilde{C},\,\mu(A^+)}],$$

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Step 4. $\mathcal{V}_\tau \subset \mathcal{A}_{\widetilde{C},\,\mu(A^+)}$:

$$\forall\,(u,v) \in \mathcal{V}_\tau \quad \exists\,\widetilde{C} \in (C_{\min}, C_{\max}) : \quad (u,v) \in \mathcal{A}_{\widetilde{C},\,\mu(A^+)}$$

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Dimensionless form of the problem

Dimensionless variables:

$$x' = \frac{x}{L}, \quad t' = v\frac{t}{L}, \qquad y(x', t') = \frac{C_A(x,t) - \overline{C}}{\overline{C}},$$

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The PFR model with one control in a dimensionless form:

$$\frac{\partial y(x',t')}{\partial t'} + \frac{\partial y(x',t')}{\partial x'} = -\boldsymbol{Da} \cdot (1 + y(x',t'))^n, \qquad (x',t') \in [0,1] \times \mathbb{R},$$

$$y(0,t') = \boldsymbol{y_0(t')} := \frac{C_{A_0}(Lv^{-1}t') - \overline{C}}{\overline{C}},$$

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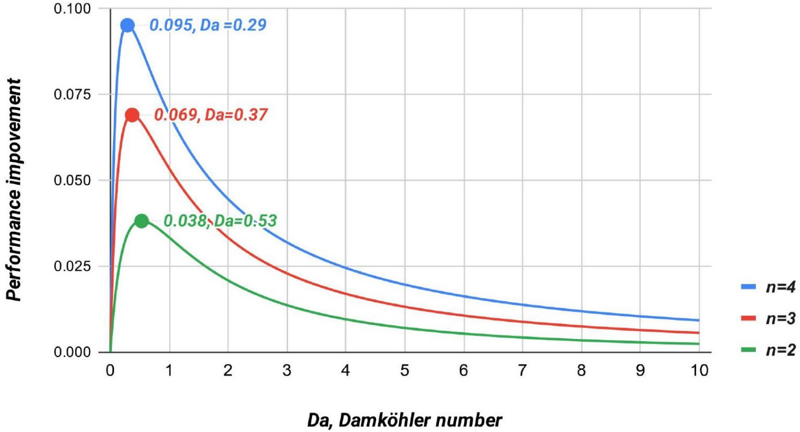
$$y(0,t') = \boldsymbol{y_0(t')} := \frac{C_{A_0}(Lv^{-1}t') - \overline{C}}{\overline{C}},$$

where $Da = k\,\tau\,\overline{C}^{\,n-1}$ is the Damköhler number:

$$\boldsymbol{Da} := \frac{\textbf{reaction time}}{\textbf{flow time}}$$

$y_0 = 0$ is a steady-state control, $\quad y_{\max} = 0.5, \quad y_{\min} = -0.5.$

Performance improvement$= J[\text{steady-state}] - J[\text{bang-bang}]$



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Conclusion and future research

Completely solved problems

- The periodic optimal control problem for a single input isothermal PFR.

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Open problems

- Non-isothermal PFR model:

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial x} + \frac{(-\Delta H)k_0}{\rho_p C_p}\exp\left(-\frac{E}{RT}\right) + \frac{4h}{\rho_p C_p d}(T_j - T),$$
$$\frac{\partial C_A}{\partial t} = -v\frac{\partial C_A}{\partial x} - k_0 C_A \exp\left(-\frac{E}{RT}\right), \quad T(0,t) = \boldsymbol{T_{in}(t)},\ C_A(0,t) = \boldsymbol{C_{A,in}(t)}$$

Conclusion and future research

Completely solved problems

- The periodic optimal control problem for a single input isothermal PFR.
- The periodic bang-bang strategies in a PFR with controlled flow-rate.

Open problems

- Non-isothermal PFR model:

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial x} + \frac{(-\Delta H)k_0}{\rho_p C_p}\exp\left(-\frac{E}{RT}\right) + \frac{4h}{\rho_p C_p d}(T_j - T),$$
$$\frac{\partial C_A}{\partial t} = -v\frac{\partial C_A}{\partial x} - k_0 C_A \exp\left(-\frac{E}{RT}\right), \quad T(0,t) = \boldsymbol{T_{in}(t)},\ C_A(0,t) = \boldsymbol{C_{A,in}(t)}$$

- Dispersed Flow Tubular Reactor model:

$$\frac{\partial C_A}{\partial t} = D_{ax}\frac{\partial^2 C_A}{\partial^2 x} - v\frac{\partial C_A}{\partial x} - kC_A^n,$$
$$C_A(0,t) = \boldsymbol{C_{A_0}(t)} + \frac{D_{ax}}{v}\frac{\partial C_A}{\partial x}\Big|_{x=0}, \qquad \frac{\partial C_A}{\partial x}\Big|_{x=L} = 0.$$