

Effect of Jacket Dynamics on Optimal Temperature Policies

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Outline

- NCO tracking for semi-batch reactors
- Reactor = Reactions + Vessel
 - Optimal *reaction* profiles
 - Optimal *reactor* inputs
- Can optimal *reactor* inputs be inferred from knowledge of optimal *reaction* profiles ?
- Batch reactor example
- Conclusions

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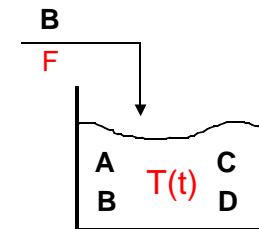
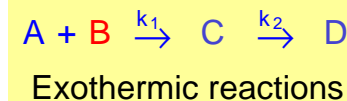
NCO tracking

B. Srinivasan, S. Palanki and D. Bonvin
[Comput. Chem. Engng, 27, 1-44 \(2003\).](#)

- The terminal-cost optimization of batch processes is characterized by
 - Discontinuous solution
 - Constraint-seeking arcs
 - Sensitivity-seeking arcs
- Optimality can be implemented using measurements by
 - Tracking active constraints
 - Driving sensitivities to zero
- The approach is
 - Straightforward for *reaction* systems
 - More difficult for industrial *reactor* systems
- This talk is on
 - Achieving the latter from the former

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Semi-batch Reaction System Optimization under Constraints



Objective: Maximize the amount of C at t_f by adjusting $F(t)$ and $T(t)$

Path constraints:

Feed rate: $F_{\min} \leq F(t) \leq F_{\max}$

Temperature: $T_{\min} \leq T(t) \leq T_{\max}$

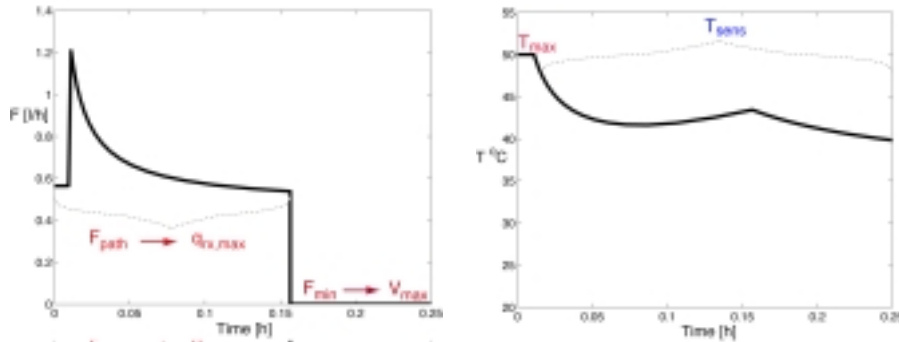
Heat production: $q_{rx}(t) \leq q_{rx,\max}$

Volume: $V(t) \leq V_{\max}$

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Semi-batch Reaction System

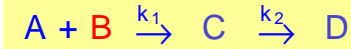
Characterization of Optimal Profiles



- Discontinuous solution with
 - Constraint-seeking arcs
 - Sensitivity-seeking arcs
- F is constraint seeking
- T is sensitivity seeking for $E_s > E_d$
- Use this qualitative information for NCO tracking

Industrial Semi-batch Reactor

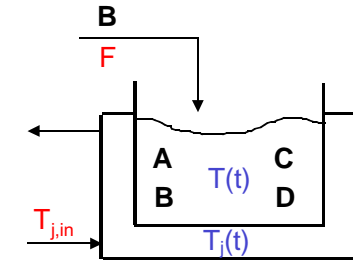
Same reactions



Exothermic reactions

Many additional effects

- Jacket dynamics
- Mass transfer limitation
- ...

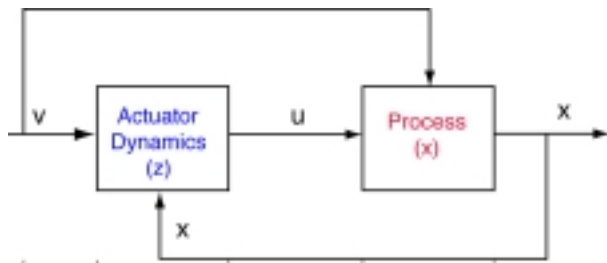


Objective: Maximize the amount of C at t_f by adjusting $F(t)$ and $T_{j,in}(t)$

Additional path constraint: Cooling temperature: $T_{j,min} \leq T_j(t) \leq T_{j,max}$

Optimal solution for F and $T_{j,in}$?

Two Optimization Problems



Problem II

$$v^* = \arg \min_{v(t)} \phi(x(t_f))$$

$$s.t. \quad \frac{dx}{dt} = F_x(x, u, v) \quad x(0) = x_0$$

$$\frac{dz}{dt} = F_z(z, x, v) \quad z(0) = z_0$$

$$u = U(z, x, v)$$

$$S_x(x, u, v) \leq 0, \quad S_z(z, x, v) \leq 0$$

$$T(x(t_f)) \leq 0$$

Problem I

$$u^* = \arg \min_{u(t)} \phi(x(t_f))$$

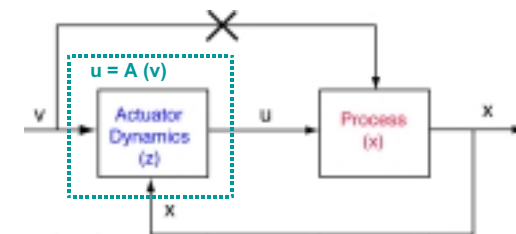
$$s.t. \quad \frac{dx}{dt} = F(x, u) \quad x(0) = x_0$$

$$S(x, u) \leq 0$$

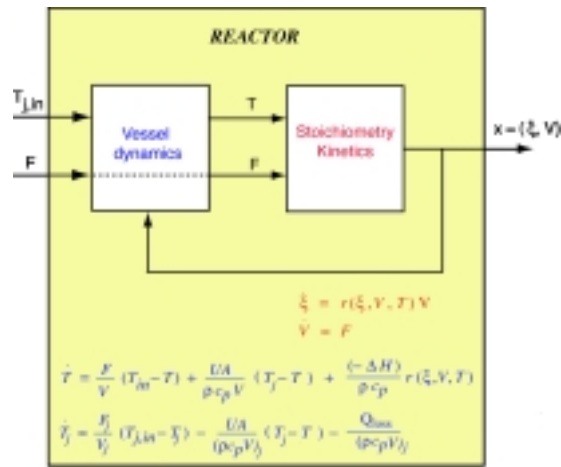
$$T(x(t_f)) \leq 0$$

Can v^* be inferred from u^* ?

- Chained invertible system
 - Chained: $F_x(x, u, v) = F(x, u)$
i.e., v has no direct effect on x, but only via u
 - Invertible: the map A can be inverted
- Theorem: For chained invertible systems, $v^* = A^{-1}(u^*)$

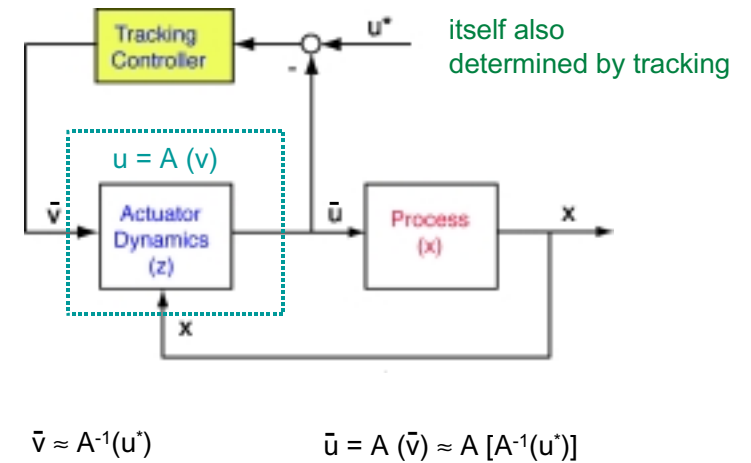


Semi-batch Reactor = Reactions + Vessel



$T_{j,in}$ affects x only via T → chained system

Approximate Inversion via Tracking



Feasibility of Inversion and Optimality

Ideal case : $\bar{u} = u^* \rightarrow$ optimal as per theorem

Best case : $\bar{u} \approx u^* \rightarrow$ near optimal

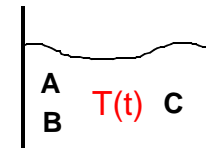
Likely case: $\bar{u} \neq u^* \rightarrow$ optimal ?

actuator dynamic constraints limit inversion

Improvements possible (illustrated with the example)

- Choose initial conditions such that these constraints are not active
- Consider error in tracking (inversion) as uncertainty
→ can be compensated with measurements via adjustment of u^* in a run-to-run fashion

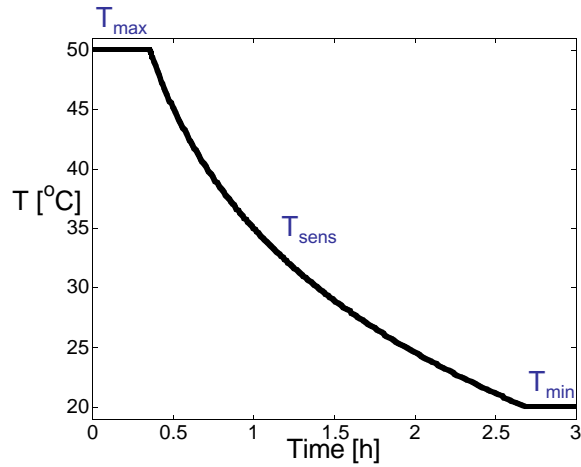
Batch Reaction System



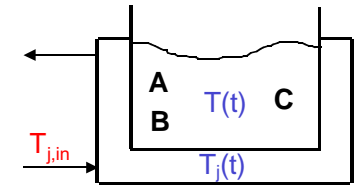
Objective: Maximize the amount of C at t_f by adjusting $T(t)$

Path constraint: Temperature: $T_{min} \leq T(t) \leq T_{max}$

Optimal Solution for the Reaction System



Batch Reactor



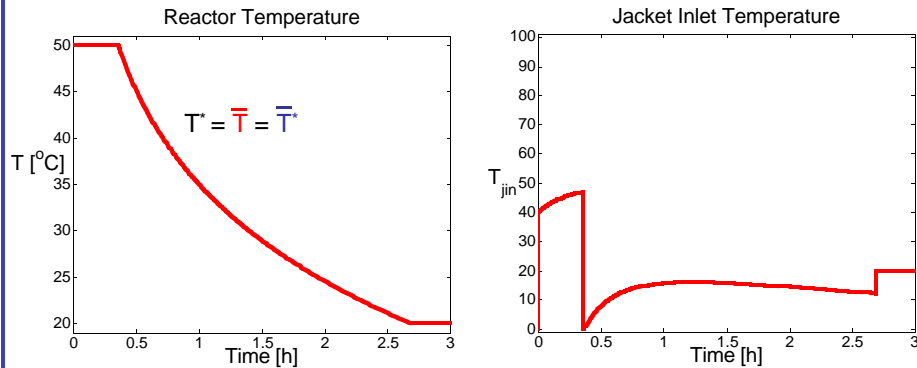
Objective: Maximize the amount of C at t_f by adjusting $T_{j,in}(t)$

Path constraint: Temperature: $T_{min} \leq T(t) \leq T_{max}$

Additional path constraint: Cooling temperature: $T_{j,min} \leq T_j(t) \leq T_{j,max}$

Optimal Solution for the Reactor

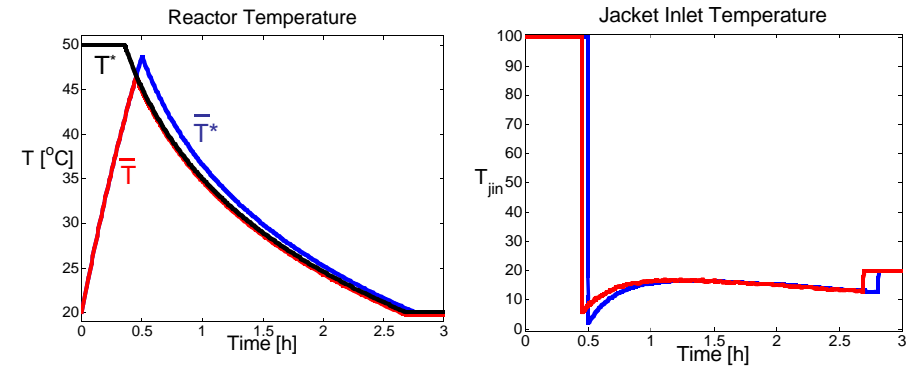
Ideal case - $T(0) = 50^\circ\text{C}$



Optimum for reaction $T^* =$ Tracking solution $\bar{T} =$ Optimum with jacket $\bar{T}^* = A(T_{j,in}^*)$

Solutions for the Reactor

Likely case - $T(0) = 20^\circ\text{C}$



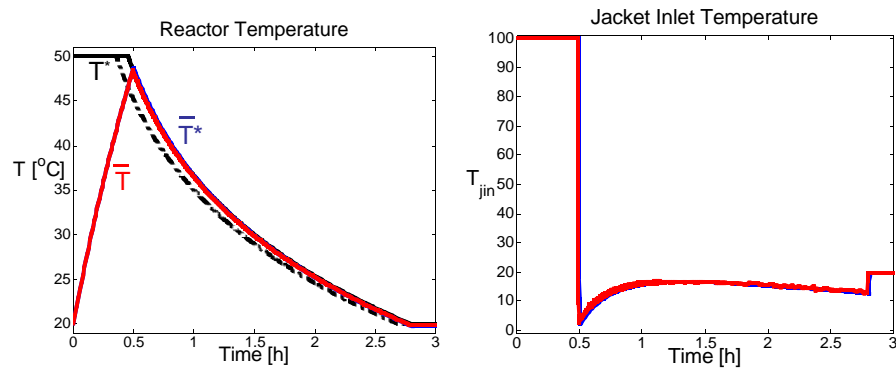
Black - optimum for reaction

Red - tracking solution

Blue - optimum with jacket dynamics

Solutions for the Reactor

$T(0) = 20^\circ\text{C}$ - with run-to-run shift of the reference



Black - optimum for *reaction* (shifted by δ)
 Red - tracking solution
 Blue - optimum with jacket dynamics

$$\frac{\Delta\phi(x(t_f))}{\Delta\delta} = 0$$

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Conclusions

- **NCO tracking: Use physical insight and characterize the optimal solution for the *reaction* part**
 - Often possible and rather intuitive
 - Can be used to determine the optimal *reactor* inputs provided the actuator dynamics can be inverted
- **Inversion of actuator dynamics**
 - If feasible, can be directly implemented
 - Otherwise, use simple run-to-run adjustments
- **This work supports our preliminary results regarding the use of NCO tracking for complex industrial systems**

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