Effect of Jacket Dynamics on Optimal Temperature Policies

B. Srinivasan and D. Bonvin
Laboratoire d'Automatique
EPFL, Lausanne, Switzerland

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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

NCO tracking

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

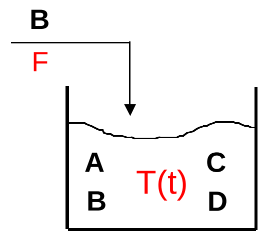
- The terminal-cost optimization of batch processes is characterized by
  - Discontinuous solution
  - Constraint-seeking arcs
  - Sensitivity-seeking arcs
- Optimality can be implemented using measurements by
  - Tracking active constraints
  - Driving sensitivities to zero
- The approach is
  - Straightforward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

Semi-batch *Reaction* System

Optimization under Constraints

$A + B \xrightarrow{k_1} C \xrightarrow{k_2} D$

Exothermic reactions



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

Path constraints:

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

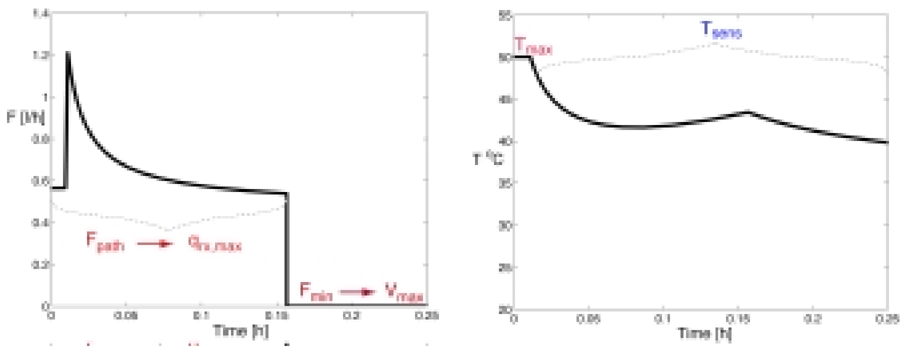
Temperature: $T_{min} \le T(t) \le T_{max}$

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

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

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*

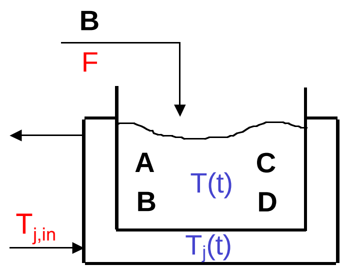
Same reactions

$A + B \xrightarrow{k_1} C \xrightarrow{k_2} D$

Exothermic reactions

Many additional effects

- Jacket dynamics
- Mass transfer limitation
- …

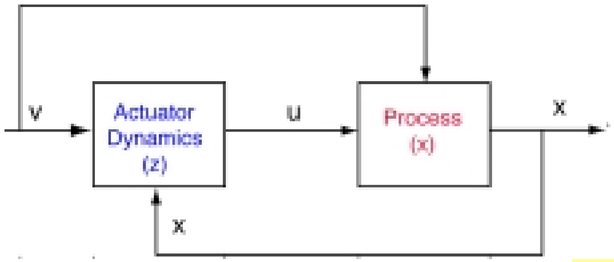


Objective: Maximize the amount of C at t_f by adjusting F(t) and $T_{j,in}(t)$

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

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

Two Optimization Problems



Problem I

$$u^* = \arg\min_{u(t)} \phi(x(t_f))$$
$$\text{s.t.}\quad \frac{dx}{dt} = F(x,u) \qquad x(0) = x_0$$
$$S(x,u) \le 0$$
$$T(x(t_f)) \le 0$$

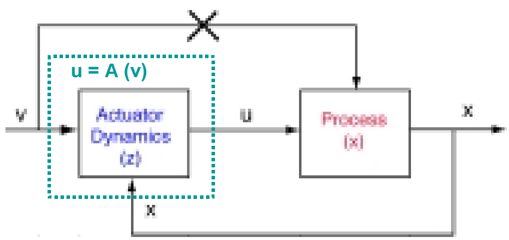
Problem II

$$v^* = \arg\min_{v(t)} \phi(x(t_f))$$
$$\text{s.t.}\quad \frac{dx}{dt} = F_x(x,u,v) \qquad x(0) = x_0$$
$$\frac{dz}{dt} = F_z(z,x,v) \qquad z(0) = z_0$$
$$u = U(z,x,v)$$
$$S_x(x,u,v) \le 0, \quad S_z(z,x,v) \le 0$$
$$T(x(t_f)) \le 0$$

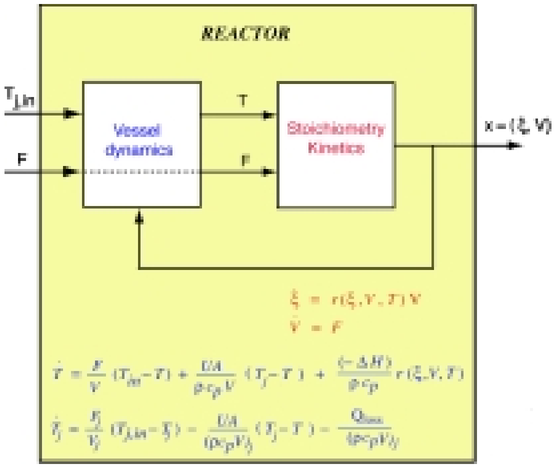
Can v^* be inferred from u^* ?

- 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, $v^* = A^{-1}(u^*)$

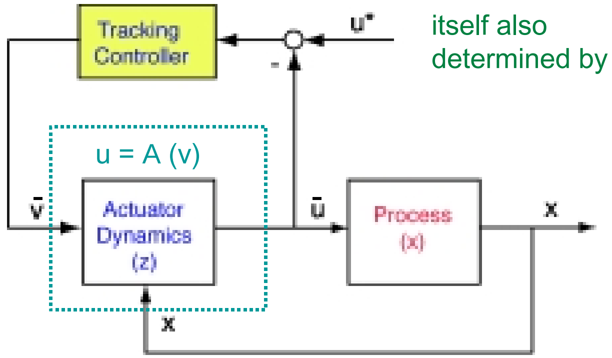


Semi-batch *Reactor* = *Reactions* + Vessel



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

Approximate Inversion via Tracking



itself also determined by tracking

$\bar{v} \approx A^{-1}(u^*)$ $\qquad$ $\bar{u} = A(\bar{v}) \approx A[A^{-1}(u^*)]$

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)

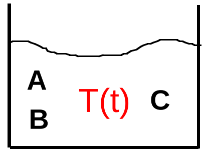
- Choose initial conditions such that these constraints are not active
- Consider error in tracking (inversion) as uncertainty

  $\rightarrow$ can be compensated with measurements via adjustment of u^*

  in a run-to-run fashion

Batch *Reaction* System

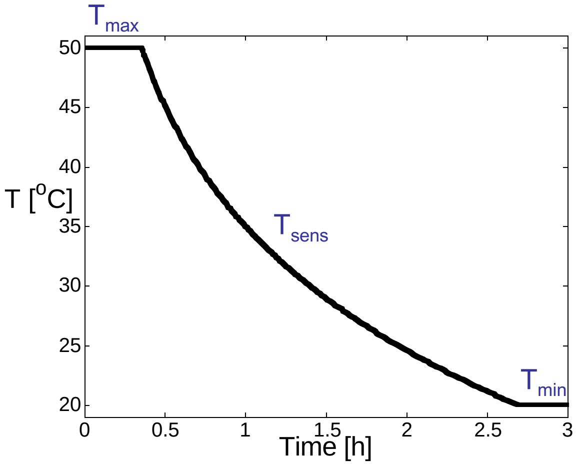
$$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} C$$



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

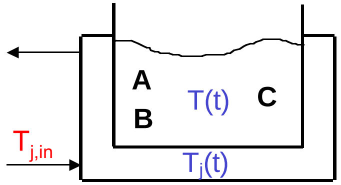
Path constraint: Temperature: $T_{min} \leq T(t) \leq T_{max}$

Optimal Solution for the *Reaction* System



Batch *Reactor*

$A + B \underset{k_2}{\overset{k_1}{\rightleftarrows}} C$



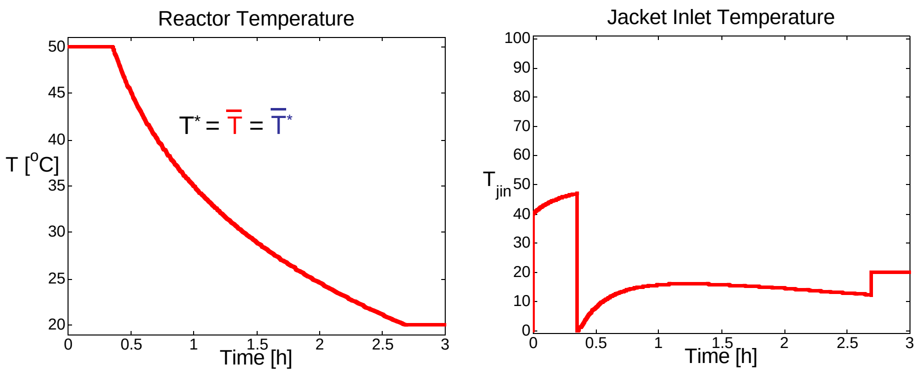
Objective: Maximize the amount of C at t_f by adjusting $T_{j,in}(t)$

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*

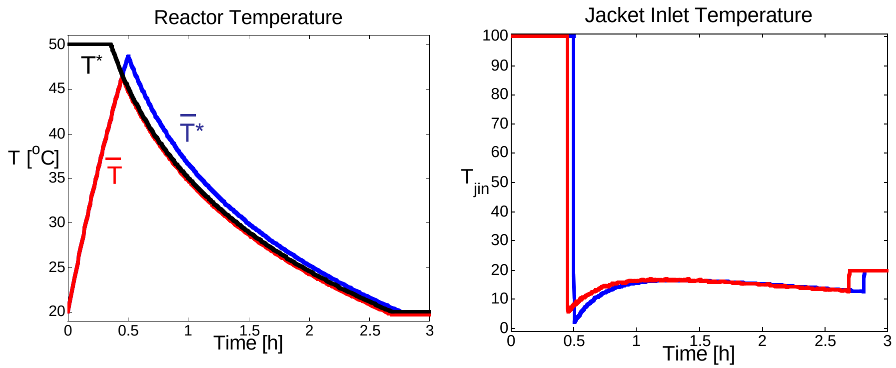
Ideal case - T(0) = 50°C



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

Solutions for the *Reactor*

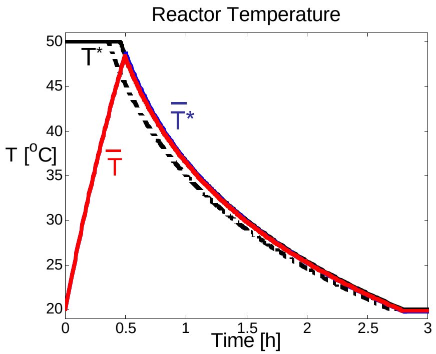
Likely case - T(0) = 20°C

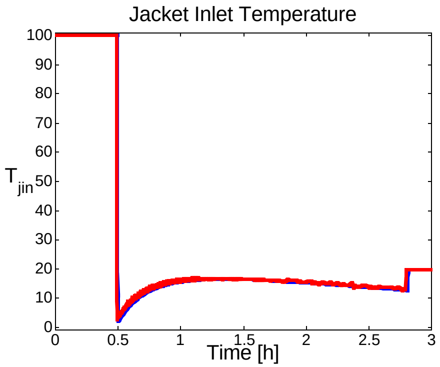


Black - optimum for *reaction*
Red - tracking solution
Blue - optimum with jacket dynamics

Solutions for the *Reactor*

T(0) = 20ºC - with run-to-run shift of the reference





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

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

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**