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Optimal Control of a Batch Reactor Using the Linearized Hamilton-Jacobi-Bellman Equation

Per Rutquist [**] **Torsten Wik** [*] **Claes Breitholtz** [*]

[*] *Department of Signals and Systems, Chalmers University of Technology, Göteborg, Sweden*
[**] *Tomlab Optimization AB, Västerås, Sweden*

AbstractIn this work we present an efficient method for solving an optimal control problem for a batch reactor, where a temperature dependent exothermic reaction takes place within a preset duration and within specified temperature bounds. The Hamilton-Jacobi-Bellman (HJB) equation corresponding to the optimal control problem is nonlinear and has infinite boundary conditions due to the state constraints (bounds on temperature and concentration), which makes it troublesome to solve. However, using a logarithmic transformation, the HJB-equation is transformed into a linear partial differential equation with zero boundary conditions. Furthermore, the problem can then be solved using variable separation such that the time-dependent part has an analytical solution and the state dependent part becomes a linear eigenvalue problem which can readily be solved using standard software.

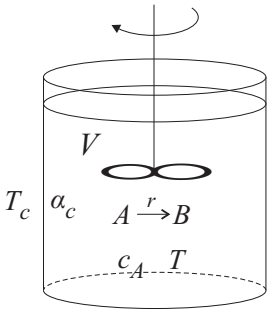

Figure 1. Illustration of the batch process.

1. INTRODUCTION

Consider the system illustrated in Figure 1, which is a batch process where a substance A reacts at a rate

$$r = k_0 e^{-\frac{E}{RT(t)}} c_A(t) \qquad \text{(mol/l/s)}$$

where E is the activation energy (J/mol), R is the ideal gas constant (J/mol/K), T is the temperature (K), k_0 is the reaction rate coefficient (1/s) and c_A is the concentration of A (mol/l). The reaction is exothermic, releasing ΔH_r Joule per mol A reacted.

The dynamics in the coolant system is ignored for simplicity and therefore we may consider the coolant temperature T_c (see Figure 1) to be the manipulated variable. The heat transfer coefficient α is assumed to be a constant parameter but in reality the transfer depends on local flows inside the reactor, coolant temperature fluctuations, flow fluctuations etc. These uncertainties and others, such as nonuniform reactions, are considered as one random disturbance that adds to the coolant temperature.

For control purposes we may write the mass and the energy balances for this system as

$$\begin{aligned} V\frac{d}{dt}c_A(t) &= -k_0 V e^{-\frac{E}{RT(t)}} c_A(t) \\ V\rho c_p \frac{d}{dt}T(t) &= \Delta H_r k_0 V e^{-\frac{E}{RT(t)}} c_A(t) \\ &\quad -\alpha_c(T(t) - T_c(t) - \Delta T_c) \end{aligned}$$

where V is the volume (l), ρ is the density (assumed unchanged by the reaction), c_p is the specific heat capacity (also assumed unchanged), and ΔT_c is the disturbance.

Selecting c_A to be the first state, T to be the second state and assuming the noise can be described by a Gaussian white noise with variance σ^2, we may write this on the form

$$\dot{x} = f(x) + G(x)(u + w), \tag{1}$$

where

$$f(x) = \begin{bmatrix} -k_0 x_1 e^{-\frac{a}{x_2}} \\ k_1 x_1 e^{-\frac{a}{x_2}} - k_2 x_2 \end{bmatrix} \quad \text{and} \quad G(x) = \begin{bmatrix} 0 \\ k_2 \end{bmatrix}$$

where $k_1 = \Delta H_r k_0/(\rho c_p)$ and $k_2 = \alpha_c/(\rho c_p V)$.

2. CONTROL PROBLEM

The batch process is operating with a cycle time t_f and at the end the concentration of A should have decreased to $c_{A,f}$ (with a corresponding produce of B). To maintain a sufficient rate of reaction the temperature should never go below $T_{\min}$ and to avoid problems of overheating it should never go above $T_{\max}$ (see Figure 2). The control problem can the be formulated as an optimization problem

$$\min_u V(x(t), t)$$

subject to Eq. (1) and

$$\begin{aligned} 0 \le x_1(t) &\le c_A(0) \\ T_{\min} \le x_2(t) &\le T_{\max} \end{aligned} \tag{2}$$

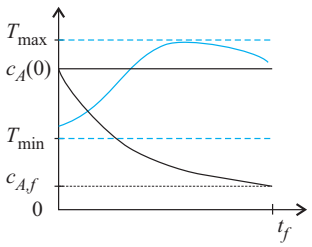

Figure 2. Constraints on the temperature and concentration trajectories.

where the cost function is

$$V(x(t),t) = \mathrm{E}\left\{\int_t^{t_f} u^2(\tau)d\tau + \gamma(x_1 - c_{A,f})^2\right\}$$

As can be seen there is no cost associated with the state trajectories although the method used would allow any such term on the form $l(x(\tau)) > 0$.

The optimal control law can be determined by solving the corresponding stochastic Hamilton-Jacobi-Bellman (HJB) equation (Dorato et al. [1995])

$$\begin{aligned} -\frac{\partial V}{\partial t} = &-\frac{\gamma}{4}(\nabla V)GG^T(\nabla V)^T + (\nabla V)f \\ &+ \frac{\sigma^2}{2}\mathrm{tr}\left[(\nabla^T\nabla V)GG^T\right] \end{aligned} \tag{3}$$

with $V \to \infty$ as $x \to \partial\Omega$, where the boundary $\partial\Omega$ is given by the state constraints (2).

3. METHOD

The nonlinearity and the infinite boundary conditions make this partial differential equation difficult to solve. However, by applying the transformation introduced by Rutquist et al. [2008] for stationary infinite horizon problems, i.e.

$$V = -\frac{2\sigma^2}{\gamma}\log(Z), \tag{4}$$

and separation of variables, i.e. $Z(t,x) = \Gamma(t)\Phi(x)$ we show that the optimal control is given by the solution to

$$\lambda\Gamma(t) = \frac{d}{dt}\Gamma(t), \tag{5}$$

which has the analytical solution $\Gamma(t) = ce^{\lambda t}$, and

$$\lambda\Phi = (\nabla\Phi)f - \frac{\sigma^2}{2}\mathrm{tr}\left[(\nabla^T\nabla\Phi)GG^T\right] \tag{6}$$

with the boundary condition

$$\Phi(x) = 0, \quad x \in \partial\Omega$$

In contrast to the difficult original HJB-equation this is a linear eigenvalue problem with zero boundary conditions that can readily be solved with standard software. The result is a family of solutions (λ_n, T_n, ϕ_n) from which the transformed cost is determined as a linear combination of the solutions for different eigenvalues, i.e.

$$Z(t,\mathbf{x}) = \sum_{n=1}^{\infty}\beta_n\exp(-\lambda_n(t_f - t))\phi_n(\mathbf{x}), \tag{7}$$

where the coefficients $\beta_n \in \mathbb{R}$ are given by the projection of the final condition

$$Z(t_f,\mathbf{x}) = \exp\left(-\frac{\gamma^2}{\sigma^2}(x_1 - c_{A,f})^2\right) \tag{8}$$

onto the space spanned by the eigenfunctions ϕ_n.

The optimal control policy can then be determined as

$$u = \frac{\sigma^2}{Z}G^T(\nabla Z)^T$$

This is illustrated by an application of the method to the reactor system described by Lagerberg and Breitholtz [1997].

REFERENCES

P. Dorato, T. C. Abdallah, and V. Cerone. *Linear Quadratic Control: An Introduction*. Prentice-Hall, 1995. ISBN 1575241560.

A. Lagerberg and C. Breitholtz. A study of gain scheduling control applied to an exothermic cstr. *Chem. Eng. Technol.*, 20:435–444, 1997.

P. Rutquist, C. Breitholtz, and T. Wik. On the infinite time solution to state-constrained stochastic optimal control problems. *Automatica*, 44:1800–1805, 2008.