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Optimal design of dispersive tubular reactors at steady-state using optimal control theory

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Abstract

This paper studies the design of optimal temperature profiles for a class of exothermic, jacketed dispersive tubular reactors under steady-state conditions and subject to maximum temperature constraints. The studied class ranges from perfectly mixed continuous stirred tank reactors to plug flow reactors. The aim is to derive the Pareto optimal set of temperature profiles for conflicting conversion and energy costs, while extracting generic features from the obtained solutions. Hereto, a four step procedure which is based on a weighted sum of both costs and which combines indirect, analytical and direct, numerical optimal control techniques, is employed. The generic features are studied (*i*) along the Pareto set by varying the weights and (*ii*) along the reactor class by adapting the dispersion level.

Key words: jacketed dispersive tubular reactor, optimal temperature profiles, Pareto curves

1 Introduction

In practice, reactor design and operation often involve an inherent trade-off between different and conflicting costs [1]. For tubular reactors, which are still important workhorses in industry, examples have been studied in the production of, e.g., (*i*) low-density polyethylene to maximise conversion, while minimising side products and compression power [2,3], and (*ii*) polystyrene

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to maximise conversion, while minimising polydispersity [4]. Apart from conversion costs and quality factors, energy recovery becomes more and more important due to increasing energy prices. Therefore, the current study provides the set of Pareto optimal solutions for conflicting conversion and energy costs. However, in contrast to optimising a finite number of parameters, this study aims at deriving analytical (and thus generic) optimal temperature profiles for a class of dispersive reactors using optimal control theory. Consequently, the obtained results allow to infer case-independent insights, which can easily be transferred to various situations. Although analytical results have been reported for plug flow reactors [5–9], results for dispersive reactors are scarce [10] due to the increased complexity arising from the second-order terms and the split Danckwerts boundary conditions. Moreover, although conceptually intuitive, the extension of previous plug flow results [8,9] to include dispersion is analytically and numerically non-trivial. Finally, the obtained open loop optimal temperature profiles can then serve as reference inputs for (i) robust closed loop controllers [11–15], for which *optimal* tracking profiles are often unknown, or for (ii) measurement based schemes [16,17]. Or, alternatively, these profiles can be an excellent starting point for purely numerical studies which employ more complex reactor models.

The organisation of the paper is as follows. Section 2 introduces the mathematical reactor model, several conflicting conversion and energy costs, as well as the constraints. Section 3 briefly repeats the optimisation framework and solution procedures, while Section 4 presents analytical and numerical results. Finally, Section 5 summarises the main conclusions.

2 Formulation of the tubular reactor optimisation problem

This section mathematically formulates the tubular reactor optimisation problem: (i) the reactor model given by ordinary differential equations, (ii) conflicting conversion and energy objectives and (iii) the constraints to be respected.

2.1 Tubular reactor model

The reactor under study is a classic tubular reactor in which an exothermic, irreversible, first-order reaction takes place. To remove the heat of reaction a surrounding jacket is present. Under the assumptions of (i) axial dispersion, (ii) steady-state conditions, (iii) perfect radial mixing, (iv) a constant density and heat capacity of the fluid, (v) a negligible heat resistance between the reactor and its jacket, and (vi) an Arrhenius law dependence of the reaction rate on the temperature, the reactor can be described by a classic 1D *dis-*

persive flow reactor (DFR) model, yielding the following set of second-order differential equations with respect to the spatial coordinate z :

$$\frac{d^2x_1}{dz^2} = \frac{v}{D_C} \frac{dx_1}{dz} - \frac{\alpha}{D_C} (1 - x_1) e^{\frac{\gamma x_2}{1+x_2}} \quad (1)$$

$$\frac{d^2x_2}{dz^2} = \frac{v}{D_T} \frac{dx_2}{dz} - \frac{\alpha\delta}{D_T} (1 - x_1) e^{\frac{\gamma x_2}{1+x_2}} - \frac{\beta}{D_T} (u - x_2) \quad (2)$$

subject to the Danckwerts boundary conditions [18]:

$$\begin{aligned} D_C \frac{dx_1}{dz} = vx_1 \quad \text{and} \quad D_T \frac{dx_2}{dz} = vx_2 \quad \text{at} \quad z = 0 \\ \frac{dx_1}{dz} = 0 \quad \text{and} \quad \frac{dx_2}{dz} = 0 \quad \text{at} \quad z = L \end{aligned} \quad (3)$$

with as state variables $x_1 = \frac{C_F - C}{C_F}$ [-] and $x_2 = \frac{T - T_F}{T_F}$ [-], the dimensionless versions of the concentration C [mol/L] and the reactor temperature T [K], and as control variable $u = \frac{T_w - T_F}{T_F}$ [-] the dimensionless version of the jacket temperature T_w [K]. T_F [K] and C_F [mol/L] are the temperature and reactant concentration of the feed stream, respectively. The jacket temperature is selected as control profile $u(z)$ to optimise the cost function(s), since this variable is in practice often used to control the reactor. D_C [m²/s] and D_T [m²/s] are the mass and energy dispersion coefficients. v [m/s] and L [m] represent the fluid velocity and the reactor length, respectively. The constants α , β , γ and δ are defined as follows:

$$\alpha = k_0 e^{\frac{-E}{RT_F}}, \beta = \frac{4h}{\rho c_p d}, \gamma = \frac{E}{RT_F}, \quad \text{and} \quad \delta = -\frac{\Delta H C_F}{\rho c_p T_F}, \quad (4)$$

with ΔH [J/kmol] the heat of reaction ($\Delta H < 0$ for an exothermic reaction), and ρ [kg/m³], c_p [J/kg K], k_0 [1/s], E [J/mol], R [J/mol K], h [W/m² K] and d [m], the fluid density, the specific heat, the kinetic constant, the activation energy, the ideal gas constant, the heat transfer coefficient, and the reactor diameter, respectively. This classic dispersive flow reactor model allows to conceptually study a class of reactors with as limiting cases the perfectly mixed continuous stirred tank reactor or CSTR (i.e., for infinite dispersion) and the plug flow reactor or PFR (i.e., for zero dispersion).

2.2 Cost functions

The conflicting objectives involve an inherent trade-off between minimising conversion and energy costs. A typical conversion cost to be minimised is the reactant concentration at the reactor outlet.

$$j_1 = C_F(1 - x_1(L)) \quad (5)$$

To incorporate energy aspects, several energy costs to be minimised can be considered. The energy cost j_2 accounts for the (scaled) net heat that has to be supplied to the reactor via the jacket. Here, energy transferred to the reactor is regarded as a cost, while energy extracted from the reactor is regarded as a benefit. Alternatively, the energy cost j_3 quantifies the heat loss at the reactor outlet, while the energy cost j_4 penalises excessive temperature deviations along the reactor length, reducing the risk on hot spots.

$$j_2 = \int_0^L \frac{\beta}{L} (u - x_2(z)) dz \quad (6)$$

$$j_3 = T_F^2 x_2^2(L) \quad (7)$$

$$j_4 = \int_0^L T_F^2 x_2^2(z) dz. \quad (8)$$

2.3 Constraints

To ensure a safe operation the reactor and jacket temperature are bounded.

$$x_{2,\min} \leq x_2(z) \leq x_{2,\max} \quad (9)$$

$$u_{\min} \leq u(z) \leq u_{\max} \quad (10)$$

3 Optimisation frame

3.1 Mathematical reformulation

Since infinite dimensional profiles have to be found, the tubular reactor optimisation problem can be (re)formulated as an *optimal control* problem:

$$\min_{u(z), z \in [0, L]} j_{\text{ws}} = (1 - A)j_{\text{conversion}} + \frac{A}{K}j_{\text{energy}} \quad (11)$$

with trade-off coefficient $A \in [0, 1]$, scaling parameter K , and cost functions:

$$j_i = h_i[\mathbf{x}(L)] + \int_0^L g_i[\mathbf{x}(z), u(z)]dz \text{ with } i = \text{conversion or energy} \quad (12)$$

subject to the system equations, the boundary conditions and the path constraints on the states and/or control:

$$\frac{d\mathbf{x}}{dz} = \mathbf{f}[\mathbf{x}(z), u(z), z] \quad (13)$$

$$\mathbf{0} = \mathbf{b}[\mathbf{x}(0), \mathbf{x}(L)] \quad (14)$$

$$\mathbf{0} \geq \mathbf{c}[\mathbf{x}(z), u(z)]. \quad (15)$$

Every solution to this *weighted sum* optimal control problem is known to be a *Pareto optimal*¹ solution for the optimisation problem with conflicting conversion and energy costs [19]. The weights (or, here, the trade-off coefficient A) can easily be linked to real economic prices. For instance, when $K = \frac{p_{\text{conversion,ref}}}{p_{\text{energy,ref}}}$ [energy/conversion] is the ratio of the reference conversion price $p_{\text{conversion,ref}}$ [money/conversion] to the reference energy price $p_{\text{energy,ref}}$ [money/energy], the reference situation is optimised for $A = 0.5$. However, as the economic situation may change, deviations can be accounted for by selecting $A = \frac{K}{K_a + K}$ with $K_a = \frac{p_{\text{conversion}}}{p_{\text{energy}}}$ [energy/conversion] the ratio of the *actual* conversion and energy prices. Varying A from 0 to 1 not only covers the entire economic spectrum, i.e., from freely available energy to worthless reaction products, but also yields an approximation of the Pareto front. However, since the weighted sum is not able to produce points in non-convex parts of the Pareto set, its convexity has to be checked afterwards.

¹ A *Pareto optimal* solution means that there exists no other feasible solution that improves one cost without worsening the other [20].

3.2 Optimisation procedure

To obtain the Pareto front with the exact (analytical) optimal control profiles, a four step procedure, which combines analytical and numerical optimal control techniques, is elaborated (see also [21]). First, *analytical expressions* for all possible arcs *are calculated* based on *indirect optimal control techniques* [22]. Second, *optimal control profiles are determined numerically* using a piecewise constant control parameterisation for a coarse grid of A -values. To tackle the boundary value problem, the software package MUSCOD-II [23] is employed, which is based on a *multiple shooting* approach [24]. In a third step the *optimal sequence* present in the numerically obtained optimal control profile *is identified* by visual inspection. This human intervention is not a restriction as automated identification procedures [25] exist. (It should be mentioned that tiny bang-bang type of arcs may be overlooked due to the coarse PWC parameterisation. However, the practical impact of these arcs is most often negligible.) Based on the identified optimal sequence the control parameterisation is each time refined using the analytical expressions found in the first step. This *analytical parameterisation* approach then leads in a fourth step to low dimensional optimisation problems with the switching positions as decision variables. These optimisations are again solved in MUSCOD-II on refined A -grids.

4 Results and discussion

Based on the conversion and energy costs from Section 2.2, three weighted sum combinations are possible: $j_1 \& j_2$, $j_1 \& j_3$, and $j_1 \& j_4$, which will be referred to as j_{ws1} , j_{ws2} , and j_{ws3} , respectively. Section 4.1 presents the results of the analytical calculations, while in Section 4.2 the numerically computed Pareto sets are discussed. Section 4.3 infers and interprets the generic features of the obtained profiles, while Section 4.4 comments on the use of the weighted sum.

4.1 Analytical arc calculation

To start, the second-order reactor model (Equations (1) and (2)) has to be adapted by introducing the gradients of the dimensionless concentration and temperature as additional state variables in order to obtain a first-order differential equation model, which fits the optimal control framework detailed above. In view of brevity, the analytical calculations for step 1 have been omitted and only the results are presented in Table 1. The arcs determined by control/state constraints are for all criteria the same. To check the possibility

of arcs inside the feasible region, the control laws have been derived based on both an explicit and implicit elimination procedure, yielding each time the same result and substantiating their correctness.

For j_{ws1} and j_{ws2} , it is found that an optimal solution is determined by active constraints, whereas for j_{ws3} also an arc inside the feasible region is possible:

$$\begin{aligned}
 u_{\text{inside}}(z) = & x_2 - \frac{\alpha\delta}{\beta}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}} - \frac{D_T}{\beta} \left\{ -\frac{v}{D_T}x_4 - \frac{v}{D_C}x_4 - 2\frac{x_3x_4}{1-x_1} \right. \\
 & + 2\left(\frac{\gamma}{(1+x_2)^2} - \frac{2}{1+x_2}\right)x_4^2 + \left[-2\frac{x_2x_3^2}{(1-x_1)^2} - 2\frac{v}{D_C}\frac{x_2x_3}{1-x_1} \right. \\
 & + 2\frac{\alpha}{D_C}e^{\frac{\gamma x_2}{1+x_2}}x_2 + x_2x_4^2\left(\frac{\gamma^2}{(1+x_2)^4} - \frac{6\gamma}{(1+x_2)^3} + \frac{6}{(1+x_2)^2}\right) \\
 & \left. \left. \cdot \left[1 - x_2\left(\frac{\gamma}{(1+x_2)^2} - \frac{2}{1+x_2}\right)\right]^{-1} \right\}. \quad (16)
 \end{aligned}$$

The types of possible arcs are identical to the ones found for the PFR [8,9]. Moreover, under the assumption that mass and heat dispersion are proportional, it can be shown that all DFR relations converge to their PFR equivalents, when dispersion tends to zero.

4.2 Numerical computation of the Pareto front

For the numerical computations the values proposed by Smets et al. [8] (see Table 2) are used as nominal parameter values. The mass and heat dispersion coefficients are assumed to be equal and the dimensionless Peclet number $Pe = \frac{vL}{D}$, indicating the importance of convective over dispersive transport, is used instead of the dispersion coefficients themselves.

In the second step, the Pareto front is approximately computed by varying the trade-off coefficient A from 0 to 1 on a coarse grid ($A \in [0 : 0.1 : 1]$) using each time a piecewise constant approximation with 50 pieces for the control u . Although apparently simple, this reactor model challenges the multiple shooting algorithm due to the presence of the dispersion terms [26]. In the third step, the different arcs are identified from the results of step 2. In the fourth step, the knowledge about the analytical arc expressions (from step 1) and the optimal arc sequence (from step 3) is combined to build analytical parameterisations with only the switching positions as degrees of freedom. These parameterisations are then optimised on a refined A -grid (i.e., $A \in [0 : 0.01 : 1]$) to obtain the exact optimal control profiles and the Pareto front.

The Pareto sets for all Peclet values ($Pe \in [0.1, 1, 2, 10, 100, 1000]$) as well as for the limiting cases, i.e., CSTR and PFR, are depicted in Figure 1 for all three criteria. The Pareto fronts are represented by the lines, while the different markers indicate the position of a certain trade-off value A . As can be seen, the continuous and convex shapes of the Pareto sets clearly illustrate the inherent and gradual trade-off between the conversion and energy costs. Hence, it can be concluded that for the current cases the weighted sum has consistently produced the convex Pareto fronts. However, an equal spread of the A -values ($A \in [0 : 0.25 : 1]$) does not necessarily lead to an equal distribution along the Pareto front. For instance for criterion j_{ws1} , although for $Pe = 100$ a more or less equal spread is obtained, a highly skew distribution is found for low Peclet numbers, e.g., $Pe = 1$. This observation indicates that the objectives in some regions of the Pareto set are much less sensitive to changes in the economic situation, then in other parts. Consequently, in these regions the optimal design and operation of the reactor will also be less sensitive to economic fluctuations.

The influence of dispersion can be summarised as follows. A smooth and continuous transition is observed over the entire range of dispersion values and convergence towards the limiting cases is found. Most of this transition is accomplished within the Peclet number range from 1 to 10. For higher values, the difference with the PFR is rather low, while for lower values, the reactor behaviour and performance is comparable to that of a CSTR. Hence, not only the different arc types converge to their PFR equivalents when dispersion tends to zero, also the numerically computed Pareto sets converge. In addition, dispersion or mixing in general is an undesired effect as it causes higher cost values and Pareto lines further away from the lower left corner.

4.3 Interpretation of the generic features

For brevity, only the optimal temperature profiles for the criterion j_{ws1} are discussed in detail. Figure 2 depicts the optimal profiles for an intermediate Peclet number $Pe = 10$. As can be seen, all the optimal reactor temperature profiles T exhibit a generic trapezoidal shape. The temperature first increases until the maximum temperature of 400 K is reached, which is then kept constant, but finally decreases again towards the reactor outlet. These trapezoidal profiles require a sequence of $u_{\max}$, u_{path} , $u_{\max}$ and $u_{\min}$ for the control variable, here, the jacket fluid temperature T_w . As predicted analytically, the optimal solution is determined by active constraints. The explanation for these generic trapezoidal reactor temperature profiles is that mainly in the first part of the reactor the reactor temperature has to be as high as possible in order to stimulate the exothermic reaction (and heat generation). Hereto, the jacket fluid temperature is at its upper limit. In the second part, generated heat is

mainly recovered by cooling the reactor as fast as possible (i.e., the jacket fluid temperature is at its lower limit). However, whenever the upper reactor temperature limit could be violated, the path constrained arc u_{path} , which enables to control the reactor temperature at its maximum value, appears in the optimal control solution and induces a constant part. The max part after the path constrained arc is in this case required to exit this u_{path} arc and to induce a negative temperature gradient, which is then decreased to 0 at the outlet by the final u_{min} piece. For the concentration, monotonically decreasing profiles are obtained as expected.

Note also the difference between the feed values ($C_F = 0.02$ mol/L and $T_F = 340$ K) and the inlet values ($C(z = 0) \approx 0.016$ mol/L and $T(z = 0) \approx 360$ K) which is induced by the Danckwerts boundary conditions and is due to the presence of a finite amount of dispersion. When looking at the corresponding Pareto plot (Figure 1), the observed negative energy cost values indicate that despite the initial amount of heat required to initiate the reaction, in the end more heat is recovered from than supplied to the reactor due to the exothermic reaction.

The bottom right plot of Figure 2 finally summarises the evolution (or bifurcation) of the jacket fluid temperature or control profile, by displaying the different switching positions along the Pareto front (i.e., when the trade-off A ranges from 0 to 1). This diagram has to be interpreted as follows. For a specific A -value the jacket fluid temperature profile can be derived by looking at a vertical line at this A -value. For instance, when A equals 0.5, the jacket fluid temperature starts with a u_{max} part of length 0.30 m, which is followed by a path constrained arc u_{path} of 0.35 m and a maximum arc u_{max} of 0.20 m, and ends with a minimum arc u_{min} of length 0.15 m. For increasing A -values, the optimal control structure varies from (i) $u_{\text{max}} - u_{\text{path}}$ over (ii) $u_{\text{max}} - u_{\text{path}} - u_{\text{max}} - u_{\text{min}}$ with decreasing u_{path} and increasing u_{min} part to (iii) $u_{\text{max}} - u_{\text{min}}$. For very high A -values the resulting temperature profiles even do not touch the upper reactor temperature limit any longer due to the high emphasis on recovering energy.

For lower Peclet numbers (see $Pe = 1$ depicted in Figure 3) rather flat profiles are obtained for the reactor temperature and concentration. However, when zooming in a (weak) trapezoidal reactor temperature profile is recognised. The differences between the value at the inlet ($z = 0$) and the feed values are larger due to the Danckwerts boundary conditions. In brief, the reactor approaches a CSTR. As displayed, the optimal control profile for the jacket fluid temperature varies along the Pareto set from $u_{\text{max}} - u_{\text{path}}$, over $u_{\text{max}} - u_{\text{path}} - u_{\text{max}} - u_{\text{min}}$ with decreasing u_{path} and increasing u_{min} zones, to $u_{\text{max}} - u_{\text{min}}$. Note that the switching position of this max-min profile remains constant over the A -range 0.73 - 0.86. Apparently, in this region touching the upper reactor temperature limit and decreasing again yields a slightly better performance than touching

the upper bound and keeping this value constant for a while before decreasing again. However, it should be noted that the sensitivity with respect to the control profile is here less pronounced due to the higher level of dispersion. For very high A -values (0.87 - 1) the switching position between $u_{\max}$ and $u_{\min}$ decreases again in order to recover more energy, and the upper reactor temperature bound is not reached any more.

For higher Peclet numbers (e.g., $Pe = 100$ depicted in Figure 4) reactor temperature and concentration profiles with steeper gradients are obtained. For the reactor temperature the typical trapezoidal profile clearly comes forward. Due to the lower dispersion, the inlet value (at $z = 0$) and the feed values hardly differ. Consequently, this reactor behaves nearly as a plug flow reactor. The optimal jacket fluid temperature profiles typically consist of a sequence $u_{\max} - u_{\min} - u_{\text{path}} - u_{\max} - u_{\min}$. The first min arc is necessary because the path constrained arc cannot be entered directly as this would require a jacket fluid temperature lower than the lower bound. When following the Pareto front for increasing A -values, it is observed that the constrained arc u_{path} (and thus the zone at the maximum reactor temperature) decreases in favour of the last min part required for cooling. This evolution again reflects the inherent trade-off between conversion induced by high temperatures and energy recovery. Finally, the generic character of these obtained trapezoidal profiles can further be evidenced by taking parametric uncertainty into account.

For the criterion j_{ws2} , also a trapezoidal reactor temperature is observed as a generic profile. The chemical interpretation is that the temperature has to be as high as possible in order to stimulate conversion, while the decrease towards the end is due to the limitation of the terminal heat loss. For the criterion j_{ws3} , a general reactor temperature profile consists of the following phases: an initial increase, followed by (i) a more or less constant part and (ii) an additional rise, which may be limited by the upper limit. Here, the explanation is that the part at the intermediate temperature reduces the energy cost, whereas the additional rise towards the end boosts the conversion. Studying the evolution along the Pareto set yields the following insights. Emphasising the energy cost induces an earlier decrease in temperature for the cost combination j_{ws2} , whereas the second temperature increase is delayed (or eventually disappears) for the cost combination j_{ws3} . The influence of dispersion is the same as before. Higher dispersion values cause smoother profiles and also higher cost values.

4.4 Remarks on the weighted sum approach

The weighted sum is one of the most common approaches for solving multiple-objective optimisation problems. This method has clear advantages, especially when the economic prices of the different objectives are known, but it also

suffers from inherent drawbacks. Points in non-convex parts of the Pareto set cannot be obtained and an even distribution of weights does not necessarily results in an even distribution along the Pareto set. Therefore, in cases without any price information, methods like Normal Boundary Intersection [27] or Normalised Normal Constraint [28] may be more efficient.

5 Conclusions

In this paper optimal temperature profiles have been computed for the optimal and safe steady-state operation of dispersive exothermic jacketed tubular reactors with conflicting conversion and energy objectives. The conceptual dispersive flow reactor model has allowed to analyse an entire class of reactors, ranging from pure plug flow to perfectly mixed reactors, and to infer generic insights. The set of Pareto optimal solutions has been constructed based on a convex weighted sum of both types of costs. To solve the related optimal control problems efficiently, a combination of indirect, analytical and direct, numerical techniques has been used in a generic four step procedure.

For all three studied cost combinations, the analytical and numerical results for the dispersive flow reactor have been found to be consistent with its limiting cases, i.e., the PFR and CSTR. In addition, it has been illustrated that increasing dispersion yields flatter profiles and larger cost values. For the first two combinations, i.e., conversion & net heat exchange, and conversion & terminal heat loss, the generic optimal reactor temperature profiles typically exhibit a trapezoidal shape. The temperature first increases until the maximum temperature is reached, then remains constant, and finally decreases again. The first two zones mainly enhance the conversion, while the third mainly decreases the energy consumption. For the combination of conversion and integral heat deviations, a generic temperature profile starts with an initial increase, followed by a more or less constant part and an additional rise, which may be limited by the upper bound. Here, the part at the intermediate temperature reduces the energy cost, while the additional rise towards the end enhances the conversion.

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Fig. 1. Total cost values (top) and Pareto front (bottom) for the criterion j_{ws1} (top), j_{ws2} (middle) and j_{ws3} (bottom).

Fig. 2. $Pe = 10$: Optimal profiles for reactor concentration (top left), reactor temperature (bottom left) and jacket fluid temperature (top right); Control switching position bifurcation diagram (bottom right).

Fig. 3. $Pe = 1$: Optimal profiles for reactor concentration (top left), reactor temperature (bottom left) and jacket fluid temperature (top right); Control switching position bifurcation diagram (bottom right).

Fig. 4. $Pe = 100$: Optimal profiles for reactor concentration (top left), reactor temperature (bottom left) and jacket fluid temperature (top right); Control switching position bifurcation diagram (bottom right).

Table 1
Analytical arc expressions.

Control	Criterion j_{ws1}	Criterion j_{ws2}	Criterion j_{ws3}
At control bounds $u_{\min}(z)$	$(T_{w,\min} - T_F)/T_F$		
$u_{\max}(z)$	$(T_{w,\max} - T_F)/T_F$		
At state bounds $u_{\text{path}}(z)$	$x_2 - \frac{\alpha\delta}{\beta}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}}$ with $x_4 = 0$ @ $x_{2,\min} = (T_{\min} - T_F)/T_F$ or @ $x_{2,\max} = (T_{\max} - T_F)/T_F$		
Inside feasible region $u_{\text{inside}}(z)$	impossible	impossible	Equation (16)

Table 2
 Process parameters.

C_F	=	0.02	$\text{mol} \cdot \text{L}^{-1}$	T_F	=	340	K
E	=	47092.5	$\text{J} \cdot \text{mol}^{-1}$	$T_{\min}$	=	280	K
k_0	=	10^6	s^{-1}	$T_{\max}$	=	400	K
K_2	=	30	$\text{mole}^{-1} \cdot \text{L}$	$T_{w,\min}$	=	280	K
K_3	=	250000	$\text{K}^2 \cdot \text{L} \cdot \text{mol}^{-1}$	$T_{w,\max}$	=	400	K
K_4	=	250000	$\text{K}^2 \cdot \text{L} \cdot \text{mol}^{-1}$	v	=	0.1	$\text{m} \cdot \text{s}^{-1}$
L	=	1	m	β	=	0.2	s^{-1}
R	=	8.3145	$\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$	δ	=	0.25	[-]

Arabic letters

A	trade-off coefficient	$[-]$
$\mathbf{b}$	vector of boundary conditions	
$\mathbf{c}$	vector of path constraints on the control/states	
C	reactant concentration	$[\text{mole} \cdot \text{L}^{-1}]$
C_F	reactant concentration in feed stream	$[\text{mole} \cdot \text{L}^{-1}]$
c_p	specific heat of reactor fluid	$[\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}]$
d	reactor diameter	$[\text{m}]$
D_C	mass dispersion coefficient	$[\text{m}^2 \cdot \text{s}^{-1}]$
D_T	heat dispersion coefficient	$[\text{m}^2 \cdot \text{s}^{-1}]$
E	activation energy	$[\text{J} \cdot \text{mole}^{-1}]$
$\mathbf{f}$	vector of system equations	
g	terminal cost part	
h	heat transfer coefficient	$[\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}]$
h	integral cost part	
j	scalar objective function	
ΔH	heat of reaction	$[\text{J} \cdot \text{kmol}^{-1}]$
k_0	kinetic constant	$[\text{s}^{-1}]$
$K_2 (K_3, K_4)$	ratio of the reference conversion price $p_{1,\text{ref}}$ to the reference energy price $p_{2,\text{ref}} (p_{3,\text{ref}}, p_{4,\text{ref}})$	$[\text{money} \cdot \text{conversion}^{-1} \cdot \text{money}^{-1} \cdot \text{energy}]$
$K_{2a} (K_{3a}, K_{4a})$	ratio of the actual conversion price p_1 to the actual energy price $p_2 (p_3, p_4)$	$[\text{money} \cdot \text{conversion}^{-1} \cdot \text{money}^{-1} \cdot \text{energy}]$
L	reactor length	$[\text{m}]$
p_1	actual price for conversion cost j_1	$[\text{money} \cdot \text{conversion}^{-1}]$
$p_2 (p_3, p_4)$	actual price for energy cost $j_2 (j_3, j_4)$	$[\text{money} \cdot \text{energy}^{-1}]$
$p_{1,\text{ref}}$	reference price for conversion cost j_1	$[\text{money} \cdot \text{conversion}^{-1}]$
$p_{2,\text{ref}} (p_{3,\text{ref}}, p_{4,\text{ref}})$	reference price for energy cost $j_2 (j_3, j_4)$	$[\text{money} \cdot \text{energy}^{-1}]$

Pe	Peclet number	$[-]$
R	ideal gas constant	$[J \cdot \text{mole}^{-1} \cdot K^{-1}]$
T	reactor fluid temperature	$[K]$
T_F	temperature of feed stream	$[K]$
T_w	jacket fluid temperature	$[K]$
u	control variable	
u	$(T_w - T_F)/T_F$, dimensionless jacket fluid temperature	$[-]$
v	reactor fluid superficial velocity	$[m \cdot s^{-1}]$
x_1	$(C_F - C)/C_F$, dimensionless reactant concentration	$[-]$
x_2	$(T - T_F)/T_F$, dimensionless reactor temperature	$[-]$
x_3	dx_1/dz , gradient of dimensionless reactant concentration	$[m^{-1}]$
x_4	dx_2/dz , gradient of dimensionless reactor temperature	$[m^{-1}]$
$\mathbf{x}$	vector of states	
z	spatial coordinate	$[m]$
Greek letters		
α	$k_0 e^{\frac{-E}{RT_F}}$	$[s^{-1}]$
β	$4h/\rho c_p d$	$[s^{-1}]$
γ	E/RT_F	$[-]$
δ	$-\Delta H C_F/\rho c_p T_F$	$[-]$
ρ	reactor fluid density	$[kg \cdot m^{-3}]$

Subscripts

$_{\min}$	value at its lower bound
$_{\max}$	value at its upper bound
$_{\text{inside}}$	value inside the feasible region
$_{\text{path}}$	value determined by path constraint
$_{\text{ws}}$	total weighted sum cost