Proceedings of the 17th World Congress
The International Federation of Automatic Control
Seoul, Korea, July 6-11, 2008

Generic Optimal Temperature Profiles for a Class of Jacketed Tubular Reactors

Filip Logist * **Peter M. Van Erdeghem** * **Ilse Y. Smets** *
Jan F. Van Impe *

* *BioTeC, Department of Chemical Engineering,*
Katholieke Universiteit Leuven,
W. de Croylaan 46, B-3001 Leuven, Belgium.
(Tel: +32-16-32.26.75, e-mail: jan.vanimpe@cit.kuleuven.be)

chemical industry, distributed-parameter systems, model-based control, optimal control, reactor control, second-order systems

Abstract: This paper deals with the optimal and safe operation of jacketed tubular reactors. Despite the existence of advanced distributed controllers, optimal steady-state reference profiles to be tracked are often unknown. In Logist et al. [2008], a procedure which combines analytical and numerical optimal control techniques, has been proposed for deriving optimal analytical (and thus generic) references, and it has been illustrated for plug flow reactors. The aim of this paper is to illustrate the general applicability of this procedure by allowing dispersion. As dispersion significantly complicates a possible solution process (due to second-order derivatives and split boundary conditions), hardly any generic results are known. Nevertheless, the dispersive plug flow reactor model is important for practice, since varying the dispersion level allows to mimic an entire reactor range, i.e., from plug flow to perfectly mixed reactors. As an example a jacketed tubular reactor in which an exothermic irreversible first-order reaction takes place is adopted. It is shown that the procedure yields generic reference solutions for (*i*) three different cost criteria, and (*ii*) different dispersion levels.

1. INTRODUCTION

Although advanced, distributed tracking controllers for tubular reactors exist (e.g., Christofides and Daoutidis [1998], Christofides [1998], Dubljevic and Christofides [2006]), the optimal steady-state references that have to be followed are often unknown. Optimal control techniques have shown to be able to provide such references (e.g., Ramagopal et al. [1983], Szwast and Sieniutycz [2001]). However, most references are computed solely numerically, i.e., without extracting generic and case independent information. Moreover, plug flow reactors have mainly been focussed on, and dispersion has been neglected. This scarcity of generic results for dispersive reactors is not surprising since the second-order terms and split boundary conditions significantly complicate the situation.

The generic analytical results obtained by Smets et al. [2002] for plug flow reactors have lead to a general procedure (Logist et al. [2008]), which allows the derivation of generic profiles based on a combination of analytical and numerical optimal control techniques. First, the set of possible arcs is calculated analytically. Second, an approximate solution is computed based on a piecewise constant representation. Afterwards, the optimal sequence of arcs is identified. Finally, the analytical arcs and the optimal sequence are combined in an analytical parameterisation of which only the switching positions have to be optimised.

The aim of the current paper is to illustrate the general character of the procedure by determining optimal and generic reference profiles for (*i*) an entire range of reactors with dispersion, and (*ii*) for different cost criteria. Section 2 formulates the optimisation problem mathematically. Section 3 briefly recalls the general procedure by Logist et al. [2008], while Section 4 presents the results. Section 5 finally summarises the main conclusions.

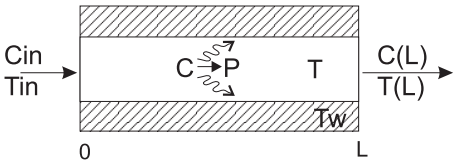

Fig. 1. Schematic view of a jacketed tubular reactor.

2. PROBLEM FORMULATION

2.1 Reactor model

The reactor under study is a classic tubular reactor (Fig. 1) in which an exothermic, irreversible, first-order reaction takes place. To remove the heat a surrounding jacket is present. When assuming (*i*) axial dispersion, (*ii*) steady-state conditions, and (*iii*) an Arrhenius law dependence of the reaction rate on the temperature, the reactor is described by the following second-order differential equations with respect to the spatial coordinate z [m]:

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

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

subject to the Danckwerts boundary conditions (Danckwerts [1953]):

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

with $x_1 = (C_{in} - C)/C_{in}$, the dimensionless concentration C [mole $\cdot$ L^{-1}], $x_2 = (T - T_{in})/T_{in}$, the dimensionless reactor temperature T [K], and $u = (T_w - T_{in})/T_{in}$, the dimensionless jacket temperature T_w [K], respectively. Since the jacket temperature T_w is not only often used in practice to control the reactor, but has also been shown to yield to most accurate references (Logist et al. [2008]), this variable is selected as the control profile $u(z)$ to be optimised. v [m/s] represents the fluid superficial velocity, while D_C [m^2/s] and D_T [m^2/s] are the mass and energy dispersion coefficients. By varying the dispersion coefficients from 0 to ∞ in this *dispersive plug flow reactor* (DPFR) model, behaviour ranging from a pure *plug flow reactor* (PFR) to a perfectly mixed *continuous stirred tank reactor* (CSTR) can be induced. In practice however, the level of dispersion is most often indicated by the dimensionless mass and energy Peclet numbers, i.e., $Pe_C = vL/D_C$ [-], and $Pe_T = vL/D_T$ [-]. The constants α, β, γ, and δ are defined as follows:

$$\alpha = k_0 e^{\frac{-E}{RT_{in}}},\ \beta = \frac{4h}{\rho C_p d},\ \gamma = \frac{E}{RT_{in}}, \delta = -\frac{\Delta H}{\rho C_p}\frac{C_{in}}{T_{in}},$$

with ΔH [J $\cdot$ kmole^{-1}] the heat of reaction ($\Delta H < 0$ for an exothermic reaction), and ρ [kg $\cdot$ m^{-3}], C_p [J $\cdot$ kg^{-1} $\cdot$ K^{-1}], k_0 [s^{-1}], E [J $\cdot$ mole^{-1}], R [J $\cdot$ mole^{-1} $\cdot$ K^{-1}], h [W $\cdot$ m^{-2} $\cdot$ K^{-1}], 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.

2.2 Cost criteria

Three different cost criteria are investigated which all involve a trade-off between a conversion cost and an energy cost. The conversion cost is measured by the reactant concentration at the outlet $C_{in}(1 - x_1(L))$. The different energy costs correspond to (*i*) the terminal heat loss, (*ii*) the penalisation of excessive reactor temperatures or hot-spots (which may cause side-reactions or catalyst decay), and (*iii*) the amount of heat exchanged between the reactor and its jacket, respectively. This yields the following three possible cost criteria:

$$J_{\text{TC}} = (1-A)C_{in}(1-x_1(L)) + A\frac{T_{in}^2}{K_1}x_2^2(L) \tag{4}$$

$$J_{\text{TIC1}} = (1-A)C_{in}(1-x_1(L)) + A\int_0^L \frac{T_{in}^2}{K_2}x_2^2 dz \tag{5}$$

$$J_{\text{TIC2}} = (1-A)C_{in}(1-x_1(L)) + A\int_0^L \frac{\beta}{K_3 L}(u-x_2)dz \tag{6}$$

with A [-] a trade-off coefficient ranging from zero to one, and K_1 [K^2 L/mole], K_2 [K^2 L/mole], and K_3 [L/mole] scaling factors, equal to 250000, 250000, and 30, respectively. The first two criteria originate from Smets et al. [2002], where they have been optimised for a plug flow reactor. The third criterion is new, and has a significant real-life value since it accounts for the reactor's net energy consumption.

2.3 Constraints

In order to avoid hazardous situations explicit bounds are imposed on the reactor and the jacket temperature.

$$x_{2,min} \leq x_2(z) \leq x_{2,max} \tag{7}$$

$$u_{min} \leq u(z) \leq u_{max} \tag{8}$$

3. GENERAL PROCEDURE

3.1 Optimal control formulation

To derive optimal profiles the problem is cast into the optimal control framework (e.g., Kirk [1970]).

$$\min_{u(z),\ z\in[0,L]} J = \underbrace{h[\mathbf{x}(L)]}_{\text{Terminal cost}} + \underbrace{\int_0^L g[\mathbf{x}(z),u(z)]dz}_{\text{Integral cost}}, \tag{9}$$

subject to the system equations for the states $\mathbf{x}$:

$$\frac{d\mathbf{x}}{dz} = \mathbf{f}[\mathbf{x}(z),u(z)] \tag{10}$$

the boundary conditions:

$$\mathbf{0} = \mathbf{I}[\mathbf{x}(0)] \tag{11}$$

$$\mathbf{0} = \mathbf{S}[\mathbf{x}(L)], \tag{12}$$

and the path constraints on the states and control:

$$\mathbf{0} \geq \mathbf{C}_1[\mathbf{x}(z)] \tag{13}$$

$$\mathbf{0} \geq \mathbf{C}_2[u(z)]. \tag{14}$$

The first-order necessary conditions for optimality are known as Pontryagin's Minimum Principle (e.g., Kirk [1970]), and involve the minimisation of a Hamiltonian:

$$\begin{aligned} \min_{u(z),\ z\in[0,L]} \mathcal{H} = {} & \boldsymbol{\lambda}^T\mathbf{f}[\mathbf{x}(z),u(z)] + g[\mathbf{x}(z),u(z)] \\ & + \boldsymbol{\mu}_1^T\mathbf{C}_1[\mathbf{x}(z)] + \boldsymbol{\mu}_2^T\mathbf{C}_2[u(z)] \end{aligned} \tag{15}$$

where $\boldsymbol{\lambda}(z) \neq \mathbf{0}$, $\boldsymbol{\mu}_1(z) \geq \mathbf{0}$, and $\boldsymbol{\mu}_2(z) \geq \mathbf{0}$ are vectors of Lagrange multipliers for the state equations and the path constraints, respectively. In literature, the vector $\boldsymbol{\lambda}$ is often called the vector of *costates*. The Lagrange multipliers $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$ are strictly positive when the corresponding inequality constraint is active, and zero otherwise.

Typically, an optimal solution consists of one or more different intervals (or *arcs*). Within each interval the control is continuous and differentiable, whereas discontinuities are allowed at the interval borders or *switching points*.

3.2 Solution procedure

The solution procedure presented in Logist et al. [2008], allows to obtain analytical and generic profiles. Hereto, both analytical and numerical optimal control techniques are combined in four successive steps.

Step 1: Analytical derivation. First, analytical expressions for all possible optimal arcs are calculated based on *indirect optimal control techniques* (Kirk [1970], Srinivasan et al. [2003]). Analytical expressions for a *control at its lower or upper bound* are readily obtained, i.e., $u(z) = u_{min}$ and $u(z) = u_{max}$. The control $u(z) = u_{path}$ to keep a *state constraint* $C_{1,i}$ active is found by repeatedly differentiating the active constraint with respect to the independent variable z: $d^k C_{1,i}[\mathbf{x}(z)]/dz^k = 0$, and replacing the derivatives by the system equations $d\mathbf{x}/dz = \mathbf{f}[\mathbf{x}(z), u(z)]$ until the control u appears explicitly. All previous derivatives (i.e., from 0 zero to $k-1$) constitute the *tangency conditions*, which also have to be fulfilled. To check whether a *control inside the feasible region* $u(z) = u_{inside}$ (i.e., when no state or control constraint is active) is possible, and to obtain its analytical expression, the costates $\boldsymbol{\lambda}$ have to be eliminated from the necessary conditions of optimality. When the Hamiltonian is affine in the control u, i.e., $\mathcal{H} = \psi + \phi u$, this elimination can be done *explicitly* by repeatedly differentiating $\phi = 0$ with respect to z, and each time substituting the state and the costate derivatives by the system equations $d\mathbf{x}/dz = \mathbf{f}[\mathbf{x}(z), u(z), z]$ and the costate equations $d\boldsymbol{\lambda}/dz = -\partial\mathcal{H}/\partial\mathbf{x}$, until the control u appears explicitly (see, e.g., Smets et al. [2002] for an example). In this case u_{inside} is often called a *singular* control arc u_{sing}. For a non-affine Hamiltonian, the costate elimination has to be performed *implicitly* using a determinant criterion (see, e.g., Srinivasan et al. [2003] for more details and Logist et al. [2008] for an example), which is more general, but involves more tedious calculations.

Step 2: Approximate numerical computation. Second, approximate piecewise constant optimal control profiles are determined numerically using the software package MUSCOD-II (Leineweber et al. [2003]), which implements a direct *multiple shooting* approach. Here, a uniform control parameterisation with 50 pieces is employed. Although apparently simple, the DPFR model challenges the multiple shooting algorithm due to the second-order dispersion terms (Kubíček and Hlaváček [1983]).

Step 3: Arc sequence identification. In a third step, the optimal sequence present in the numerically obtained optimal control profile is identified by visual inspection. This human intervention is, however, not a restriction as an automated identification procedure (Schlegel and Marquardt [2006]) can also be employed.

Step 4: Exact computation with an analytical parameterisation. 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 a low dimensional optimisation problem with the switching positions between the different intervals as decision variables. These optimisations are again solved in MUSCOD-II. The resulting control profiles now provide the exact solution to the optimal control problem, since the optimal analytical relations are exploited. Alternatively, after having identified the optimal sequence, Schlegel and Marquardt [2006] have optimised analytical parameterisations employing low-dimensional piecewise linear instead of the optimal analytical expressions. This approach obviously introduces approximation errors but allows to deal also with large-scale systems.

Table 1. Process parameters.

C_{in}	=	0.02 mole $\cdot$ L^{-1}	T_{max}	=	400 K
E	=	47092.5 J $\cdot$ mole^{-1}	$T_{w,min}$	=	280 K
k_0	=	10^6 s^{-1}	$T_{w,min}$	=	400 K
L	=	1 m	v	=	0.1 m $\cdot$ s^{-1}
T_{in}	=	340 K	β	=	0.2 s^{-1}
T_{min}	=	280 K	δ	=	0.25 [-]

4. RESULTS

This section discusses the results when the general procedure is applied to the three different cost criteria for different dispersion levels. As mass and heat dispersion are often in the same order of magnitude, equal mass and heat dispersion is assumed, indicated by a single Peclet number Pe. The remaining parameter values originate from Smets et al. [2002], and are summarised in Table 1.

To fit into the optimal control framework mentioned above, the second-order reactor model (1) and (2) has to be adapted by introducing the gradients of the dimensionless concentration and temperature as additional state variables $x_3 = dx_1/dz$ and $x_4 = dx_2/dz$, in order to obtain the following system of first-order differential equations:

$$\frac{dx_1}{dz} = x_3 \tag{16}$$

$$\frac{dx_2}{dz} = x_4 \tag{17}$$

$$\frac{dx_3}{dz} = \frac{v}{D_C}x_3 - \frac{\alpha}{D_C}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}} \tag{18}$$

$$\frac{dx_4}{dz} = \frac{v}{D_T}x_4 - \frac{\alpha\delta}{D_T}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}} - \frac{\beta}{D_T}(u-x_2) \tag{19}$$

and corresponding boundary conditions:

$$\begin{aligned} D_C x_3 &= v x_1 \quad \text{and} \quad D_T x_4 = v x_2 \quad \text{at} \quad z = 0 \\ x_3 &= 0 \quad \text{and} \quad x_4 = 0 \quad \text{at} \quad z = L. \end{aligned} \tag{20}$$

4.1 Step 1: analytical results

As mentioned, step 1 consists of deriving all possible optimal arcs. Since the constraints (7) and (8) apply to all three cost criteria, the arcs resulting from active constraints are the same for all three cases: u_{min}, u_{max}, and $u_{path} = x_2 - \frac{\alpha\delta}{\beta}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}}$. Here, the first two originate directly from the control bounds, while the latter is found after two differentiations of the state constraint (7). Apart from being at a bound ($x_{2,min}$ or $x_{2,max}$), also the *tangency condition* from the first constraint derivative has to be satisfied, i.e., $x_4 = 0$. This condition is intuitive, as on a maximum/minimum reactor temperature interval the temperature gradient has to equal zero.

To check the possibility of arcs inside the feasible region, the Hamiltonians for all three criteria have to be constructed. Because the system is affine in the control u, and

Table 2. Analytical relations for the different cost criteria.

Control		Criterion J_{TC}	Criterion J_{TIC1}	Criterion J_{TIC2}
At control bounds (8)	$u_{min}(z)$	$u_{min} = (T_{w,min} - T_{in})/T_{in}$		
	$u_{max}(z)$	$u_{max} = (T_{w,max} - T_{in})/T_{in}$		
At state bounds (7)	$u_{path}(z)$	$x_2 - \frac{\alpha\delta}{\beta}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}}$ with $x_4 = 0$		
		@ $x_{2,min} = (T_{min} - T_{in})/T_{in}$ or @ $x_{2,max} = (T_{max} - T_{in})/T_{in}$		
Inside feasible region	$u_{inside}(z)$	impossible	Equation (21)	impossible

this control appears at most affinely in an integral cost, all Hamiltonians are also affine in this variable. Hence, the elimination of the costates can be performed explicitly. For brevity, the symbolic calculations have been omitted, and only the results are presented in Table 2. Apparently, an arc inside the feasible region is impossible for the criterion J_{TC} since this would require all costates to be identically equal to zero, which is prohibited. The second criterion J_{TIC1} on the other hand, does yield an explicit relation for a control arc inside the feasible region:

$$\begin{aligned} u_{inside} = x_2 - \frac{\alpha\delta}{\beta}(1-x_1)e^{\frac{\gamma x_2}{1+x_2}} - \frac{D_T}{\beta}\Bigg\{ & -\frac{v}{D_T}x_4 \\ & +2\left(\frac{\gamma}{(1+x_2)^2} - \frac{2}{1+x_2}\right)x_4^2 - \frac{v}{D_C}x_4 - 2\frac{x_3 x_4}{1-x_1} \\ & +\Bigg[-2\frac{x_2 x_3^2}{(1-x_1)^2} - 2\frac{v}{D_C}\frac{x_2 x_3}{1-x_1} + 2\frac{\alpha}{D_C}e^{\frac{\gamma x_2}{1+x_2}}x_2 \\ & +x_2 x_4^2\left(\frac{\gamma^2}{(1+x_2)^4} - \frac{6\gamma}{(1+x_2)^3} + \frac{6}{(1+x_2)^2}\right)\Bigg] \\ & \cdot\left[1 - x_2\left(\frac{\gamma}{(1+x_2)^2} - \frac{2}{1+x_2}\right)\right]^{-1}\Bigg\} \end{aligned} \tag{21}$$

Finally, for the third criterion J_{TIC2}, the elimination procedure does not provide a relation for a control inside the feasible region, since it results in the identity $0 = 0$.

4.2 Step 2, 3 and 4: numerical results

In a second and a third step, the piecewise constant control is optimised, and the optimal arc sequence is identified. Finally, the switching positions of an analytical parameterisation based on the analytical relations and the optimal sequence, are optimised to yield the exact optimal solution. With a trade-off value A equal to 0.5, the resulting optimal concentration C, reactor temperature T, and jacket fluid temperature T_w profiles are each time displayed in Figs 2, 3, and 4 for the three criteria. The effect of dispersion is indicated by the Peclet number Pe.

Criterion J_{TC}. When looking at the criterion J_{TC} (Fig 2), trapezoidal reactor temperature profiles appear to be optimal for high Peclet values (e.g., $Pe = 100$). This behaviour is similar to that of a plug flow reactor. The generic explanation is that the reactor has to be heated as fast as possible, until the upper temperature limit of 400 K is reached. Then, this temperature is maintained for a certain length, and finally it is lowered towards the outlet. The first two phases are intended to increase conversion, whereas the latter decreases the terminal heat loss. The resulting control sequences are $u_{max} - u_{min} - u_{path} - u_{max} - u_{min}$. Here, the first *min* part is required because the path constrained arc cannot be entered directly, since this would require a control value beneath the lower bound. The second *max* part on the other hand, induces a negative gradient which has be brought to zero at the outlet.

Increasing the level of dispersion (i.e., decreasing the Peclet number) has two effects. First, the profiles are smoothed, and second, the differences between the feed values $C_{in} = 0.02$ mole/L and $T_{in} = 340$ K, and the inlet values $C(z=0)$ and $T(z=0)$ increase due to the Danckwerts boundary conditions. For low Peclet numbers (e.g., $Pe = 1$), the behaviour approximates that of a perfectly mixed CSTR. For these situations the upper reactor limit is not reached anymore, and the optimal control is of the $u_{max} - u_{min}$ type.

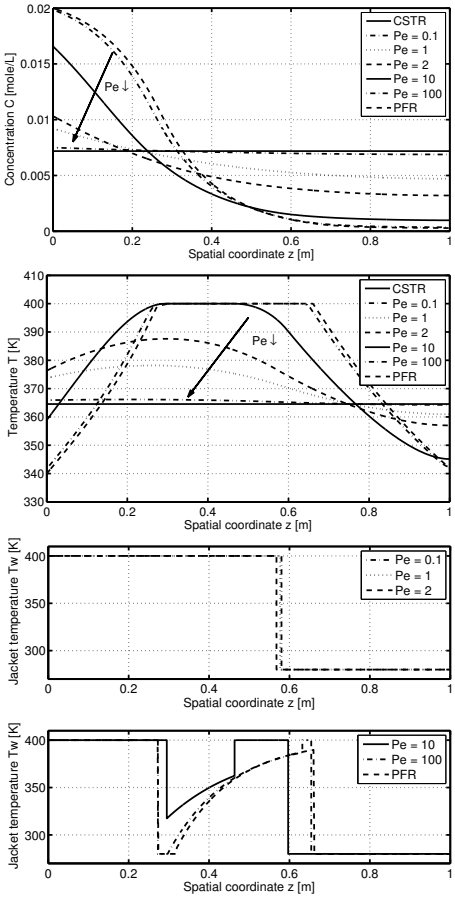

Fig. 2. Criterion J_{TC}: Optimal profiles for different Peclet numbers: concentration C (top), reactor temperature T (middle), and jacket temperature T_w (bottom).

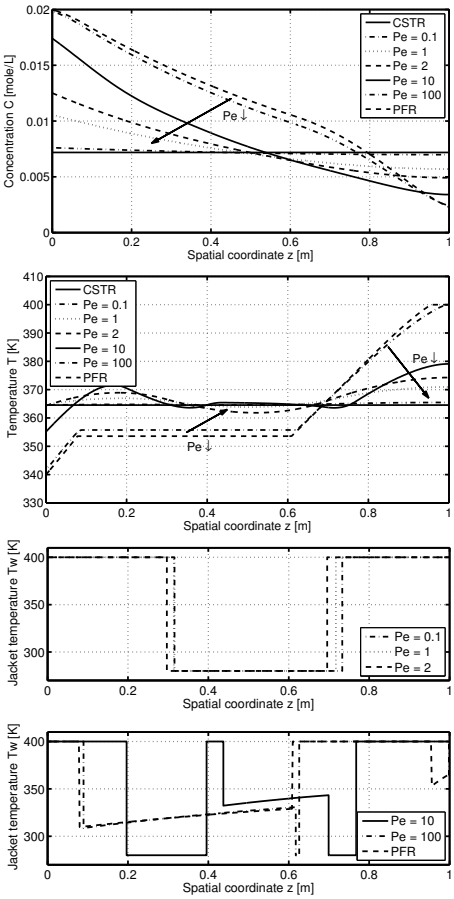

Fig. 3. Criterion J_{TIC1}: Optimal profiles for different Peclet numbers: concentration C (top), reactor temperature T (middle), and jacket temperature T_w (bottom).

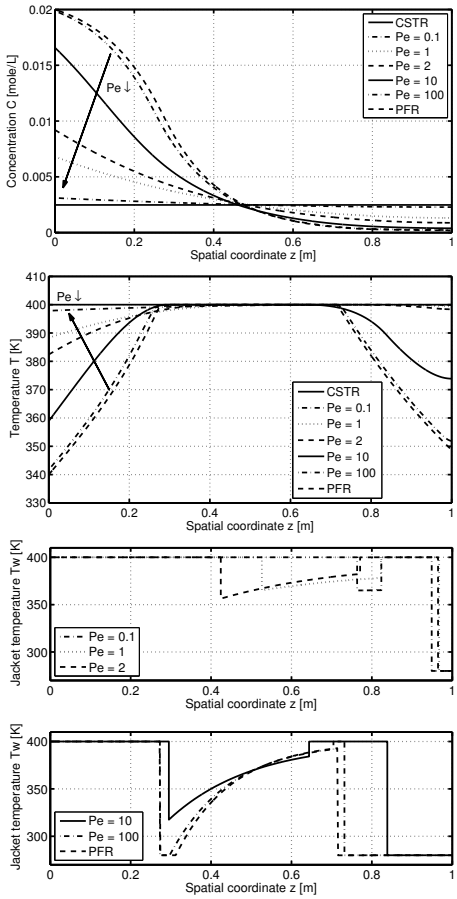

Fig. 4. Criterion J_{TIC2}: Optimal profiles for different Peclet numbers: concentration C (top), reactor temperature T (middle), and jacket temperature T_w (bottom)

Criterion J_{TIC1}. A similar analysis is possible for the criterion J_{TIC1}. Here, for high Peclet values (e.g., $Pe = 100$) the reactor temperature has to be brought to an intermediate level, which has to be kept constant for a certain length. Then, towards the outlet the temperature is raised again, until the upper bound is attained. The explanation is that in the first part the temperature is limited by the penalisation of high temperatures, whereas towards the end, an additional temperature rise is allowed to increase conversion. Increasing dispersion increases the intermediate temperature level, but reduces the second temperature rise. Finally, for low Peclet values the entire profile levels to the constant value that is also encountered in a CSTR. The control sequences encountered are more complex, and exhibit an arc inside the feasible region for high Peclet values (e,g., $Pe = 100$). For low Peclet values (e.g., $Pe = 1$), however, this arc disappears.

Criterion J_{TIC2}. For this criterion, similar trapezoidal temperature profiles as for J_{TC} are obtained. Again, the temperature is first increased as fast as possible by supplying heat in order to stimulate conversion. When the upper temperature limit is reached, this value is maintained. Here, conversion is increased, while the energy cost is lowered because heat is extracted. Finally, additional heat is extracted by cooling towards the outlet. However, when dispersion is increased, higher reactor temperatures are observed in order to counter the decreased conversion rate due to mixing effects. The control sequence is also similar to that of the first criterion: $u_{max} - u_{min} - u_{path} - u_{max} - u_{min}$. Here, the first *min* part vanishes for low Peclet values.

Total cost values. The above mentioned procedure has been repeated for a range of trade-off values A, and the resulting total cost values for all three criteria are depicted in Fig. 5. Here, low A-values emphasise conversion, whereas high A-values penalise energy costs. Clearly, for all criteria and all trade-off values, dispersion is undesired as it causes an increase in the total cost.

5. CONCLUSIONS

In this paper generic optimal temperature profiles have been derived for the dispersive plug flow reactor model. By varying the dispersion coefficient reactors ranging from perfectly mixed CSTRs to pure PFRs have been investigated. Despite the increased complexity due to the second-order terms and split Danckwerts boundary conditions, the four step procedure introduced in Logist et al. [2008] for plug flow reactors, has been shown to be still applicable. Hereto, the set of possible optimal control arcs is first derived analytically. Second, an approximate piecewise constant optimal profile is computed numerically. From this approximation the optimal control arc sequence is identified in a third step. Employing this optimal sequence

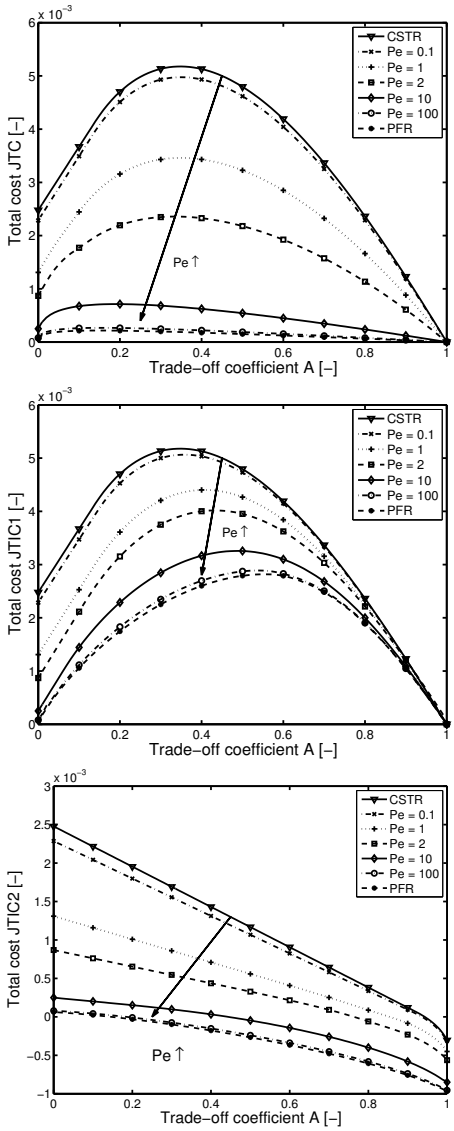

Fig. 5. Total cost values for different trade-off values and Peclet numbers: J_{TC} (top), J_{TIC1} (middle), and J_{TIC2} (bottom).

and the analytical expressions, results in an analytical parameterisation, where only the switching positions have to be optimised.

Results for the class of reactors have been presented for three cost criteria, which all involve a trade-off between a conversion and an energy cost. Each time the optimal reference profiles have been interpreted chemically, and generic knowledge has been inferred.

For the first and the third criterion trapezoidal reactor temperature profiles have been found to be optimal. Here, the temperature is increased until the upper limit is reached, then this temperature has to be kept constant for a certain interval, before decreasing again towards the outlet. The first two phases mainly stimulate conversion whereas the last reduces the energy cost. For the second criterion, it is important to maintain a more or less constant intermediate reactor temperature, which may be increased towards the end. This intermediate value limits the energy cost, whereas the possible additional temperature rise induces a conversion boost.

Although dispersion has a smoothing effect, the generic features remain the same. Hence, all these generic profile features can serve as references for distributed tracking controllers. In addition, a gradual evolution of the total cost values has been observed towards the two extremes, i.e., the PFR and the CSTR. However, dispersion is undesired as it induces higher cost values.

ACKNOWLEDGEMENTS

Work supported in part by Projects OT/03/30 and EF/05/006 (Center-of-Excellence Optimization in Engineering) of the Research Council of the Katholieke Universiteit Leuven, and by the Belgian Program on Interuniversity Poles of Attraction, initiated by the Belgian Federal Science Policy Office. The scientific responsibility is assumed by its authors.

REFERENCES

P.D. Christofides. Robust control of parabolic PDE systems. *Chemical Engineering Science*, 53:2949–2965, 1998.

P.D. Christofides and P. Daoutidis. Robust control of hyperbolic PDE systems. *Chemical Engineering Science*, 53:85–105, 1998.

P.V. Danckwerts. Continuous flow systems. *Chemical Engineering Science*, 2:1–13, 1953.

S. Dubljevic and P.D. Christofides. Predictive output feedback control of parabolic partial differential equations. *Industrial and Engineering Chemistry Research*, 45:8421–8429, 2006.

D.E. Kirk. *Optimal Control Theory: an Introduction*. Prentice Hall, Englewood Cliffs, New Jersey, 1970.

M. Kubíček and V. Hlaváček. *Numerical Solution of Nonlinear Boundary Value Problems with Applications*. Prentice-Hall, Englewood Cliffs, New Jersey, 1983.

D.B. Leineweber, A. Schäfer, H.G. Bock, and J.P. Schlöder. An efficient multiple shooting based reduced SQP strategy for large-scale dynamic process optimization. Part II: Software aspects and applications. *Computers and Chemical Engineering*, 27:167–174, 2003.

F. Logist, I.Y. Smets, and J.F. Van Impe. Derivation of generic optimal reference temperature profiles for steady-state exothermic jacketed tubular reactors. *Journal of Process Control*, 18:92–104, 2008.

A. Ramagopal, A. Kumar, and S.K. Gupta. Optimal temperature profiles for nylon 6 polymerization in plug-flow reactors. *Journal of Applied Polymer Science*, 28: 2261–2279, 1983.

M. Schlegel and W. Marquardt. Detection and exploitation of the control switching structure in the solution of dynamic optimization problems. *Journal of Process Control*, 16:275–290, 2006.

I.Y. Smets, D. Dochain, and J.F. Van Impe. Optimal temperature control of a steady-state exothermic plug flow reactor. *AIChE Journal*, 48:279–286, 2002.

B. Srinivasan, S. Palanki, and D. Bonvin. Dynamic optimization of batch processes I. Characterization of the nominal solution. *Computers and Chemical Engineering*, 27:1–26, 2003.

Z. Szwast and S. Sieniutycz. Optimal temperature profiles for parallel-consecutive reactions with deactivating catalyst. *Catalysis Today*, 66:461–466, 2001.