# Cocurrently-Cooled Fixed-Bed Reactors: A Simple Approach to Optimal Cooling Design

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Wall-cooled fixed-bed reactors are commonly used in industrial plants to carry out highly exothermic reactions. Due to the presence of important heat effects, these units present the well known problems of pronounced maxima in the axial temperature profile (hot spots) and high parametric sensitivity.

The safe design of these reactors has been intensively studied during the last decades. Two extensive reviews have recently been published on the subject by Puszyński et al. (1981) and Froment (1984). Except for the works related to autothermal reactors, most researchers assume that the coolant temperature profile is constant. Only recently has attention been paid to the influence of the coolant-zone design on reactor operation. Luss and Medellin (1972) and Akella and Lee (1983) studied the behavior of countercurrently-cooled nonisothermal tubular reactors, while the cocurrent scheme has been studied by, among others, Degnan and Wei (1979), Soria López et al. (1981), and Hosten and Froment (1986). More complex coolant flow configurations have been studied by Smith and Banchero (1973) and McGreavy and Dunbobbin (1978).

In a recent contribution, Borio et al. (1989) analyzed, comparatively, three basic cooling schemes: countercurrent, cocurrent and perfectly mixed coolant. They concluded that for equivalent production rates, the cocurrent operation is the one which yields the lowest values for the maximum temperature and parametric sensitivity, provided an adequate selection for the coolant flow rate can be made.

In the present work, following the same guidelines, a simple expression is developed to predict the coolant flow rate value leading to conditions of maximum attainable safety (minimum hot spot and low parametric sensitivity). This analytical tool allows the solution of this optimization problem without the need to resort to a laborious iterative simulation of the unit.

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## Definition of the Safety Problem

The reactor model presented by Borio et al. (1989) will be used here. They analyzed a multitubular fixed-bed reactor for phthalic anhydride production, cooled by means of a liquid of very high thermal conductivity. The highly exothermic reaction of o-xylene oxidation with excess air is assumed to be a pseudo-first-order irreversible one. Finally, as often occurs in practice, both the temperatures of the reactants and of the coolant medium are considered to be equal at the inlet of the reaction section.

The above described model results in the following set of ordinary differential equations, where the values of the parameters needed in the calculations are those reported by van Welsenaere and Froment (1970) and Soria López et al. (1981):

$$-\frac{dp_A}{dz} = A\, p_A\, k_\infty \exp(-a/T) \quad (1)$$

$$\frac{dT}{dz} = B\, p_A\, k_\infty \exp(-a/T) - C\,(T - Tc) \quad (2)$$

$$\frac{dTc}{dz} = D\,(T - Tc) \quad (3)$$

where, for

$$z = 0 \quad p_A = p_{A_0}, \quad T = Tc$$

$$z = j \quad Tc = Tc_j, \quad \text{with} \begin{cases} j = 0 & \text{cocurrent} \\ j = L & \text{countercurrent} \end{cases}$$

Borio et al. (1989) solved Eqs. 1–3 together with the set of three coupled differential equations for the parametric sensitivity at each point of the reactor length. From the simulation results they demonstrated that the cocurrent arrangement exhibits lower hot spots and lower parametric sensitivities than those found in the alternative coolant schemes, yielding shorter reactors and a safer operation. Also, there are two particular values of the coolant flow rate, both in the cocurrent scheme, which, for a given production rate, respectively minimize the maximum reactant temperature and the maximum parametric sensitivity.

All this is illustrated in Figure 1, where the maximum temperature in the reactor tube ($T_M$) and the extreme in the axial profile of the reactant temperature sensitivity, with respect to the inlet coolant temperature ($S^*$), are plotted against $Wc^{-1}$. A first inspection reveals that the minimum of the $T_M$ curve is much more pronounced than that of the $S^*$ curve. Due to this, the reactor should operate ideally at the value of $Wc$ indicated as $Wc_{opt}$, provided that it yields both minimum $T_M$ and an $S^*$ very close to its lowest value, $S^*_m$. Therefore, in a first approach, $Wc_{opt}$ can be defined as the optimal design for the cooling side from the safety standpoint.

However, the calculation of $Wc_{opt}$ is not a trivial problem. In fact, a different $Wc_{opt}$ is found for each set of values for the reactor size and the variables which determine the production rate ($G_g$, $p_{A_o}$, and $x_L$). To illustrate this, the influence of the reactor length on $Wc_{opt}$ is shown in Figure 2 for the same production requirements. In principle, a numerical solution to the problem is needed, e.g., by means of an optimization algorithm which, at each step, would require a reactor simulation in order to evaluate the objective function, $T_M$. Moreover, the fact of imposing a given production rate gives rise to a boundary value problem, introducing an additional complexity to the calculation.

In the following, a method is described which constitutes a direct and simple way to approximate this problem. As a previous step, the relationship between the minimum $T_M$ and the isothermicity conditions, which is necessary to the present development, will be discussed.

## Theoretical Minimum for $T_M$

Assume a tubular reactor where a first-order reaction takes place and where its dimensions, the flow rate of reactants, and

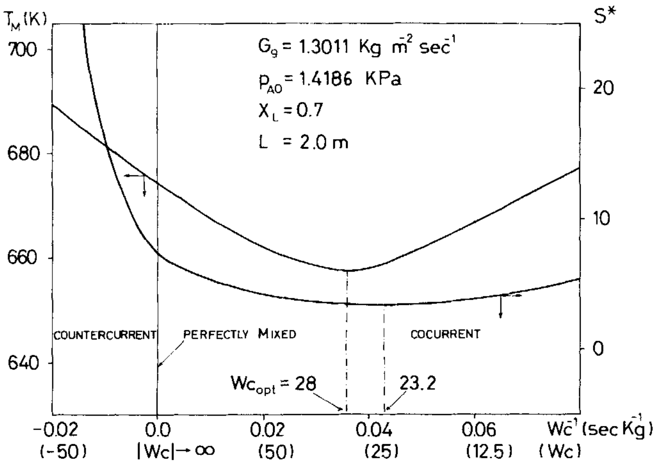


**Figure 1. $T_M$ and $S^*$ vs. $Wc^{-1}$ curves at conditions of constant production rate for a fixed reactor length.**

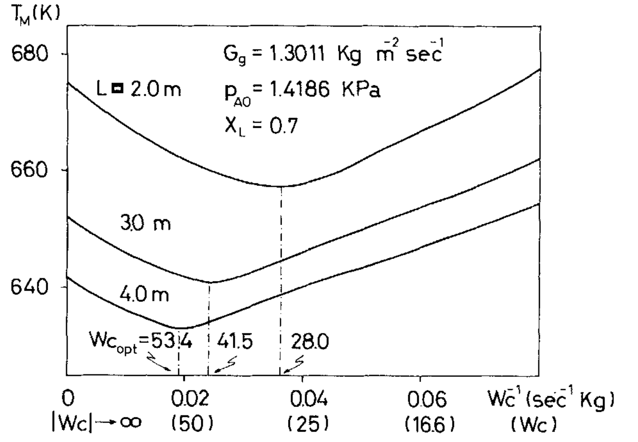


**Figure 2. $T_M$ vs. $Wc^{-1}$ curves at conditions of constant production rate for different reactor lengths.**

the outlet conversion are given. If the desired objective is to minimize $T_M$, it can be easily proved that the isothermal temperature profile is the optimum one.

For the particular case of wall-cooled fixed-bed reactors, Degnan and Wei (1979) deduced that the isothermal operation is only possible: a) under a cocurrent scheme and b) if independent preheating of the reactant stream is available ($T_o \neq Tc_o$). In this case, from Eqs. 1–3 the theoretical isothermal operation will be held at:

$$T_i = \frac{a}{\ln (A\, k_\infty / D)} \tag{4}$$

For the system to work under this isothermal operation, however, it is also necessary to fix the following inlet conditions:

$$T_o = T_i \tag{5}$$

$$Tc_o + \frac{BD}{AC} p_{A_o} = T_i \tag{6}$$

In order to select, from the infinite number of theoretically possible isothermal operations, the one which yields a given outlet conversion, $x_L$, the parameter $D$ in Eq. 4 must satisfy the following expression:

$$D = \frac{1}{L} \ln \left[ \frac{1}{1 - x_L} \right] \tag{7}$$

Therefore, any nonisothermal operation giving the same conversion, $x_L$, for the same value of the residence time of the reactants ($A \cdot L$ = constant), must exhibit a portion of the reactor length with temperatures higher than $T_i$. From this analysis it can be concluded that with the industrial designs which do not include the possibility of independently preheating the reactant stream, the problem of minimizing $T_M$ is equivalent to reducing to a minimum the difference between $T_M$ and $T_i$.

## Approximation to the Maximum Safety Design

The problem of an optimum cooling design from the safety standpoint, will be discussed within the framework of the nonisothermal operation, which is characteristic of industrial condi-

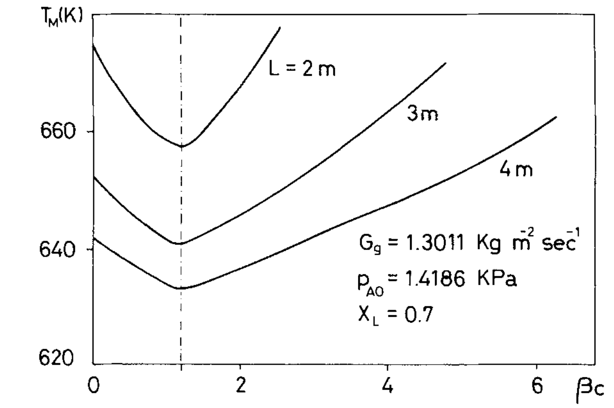


**Figure 3. $T_M$ vs. $\beta c$ curves at conditions of constant production rate for different reactor lengths.**

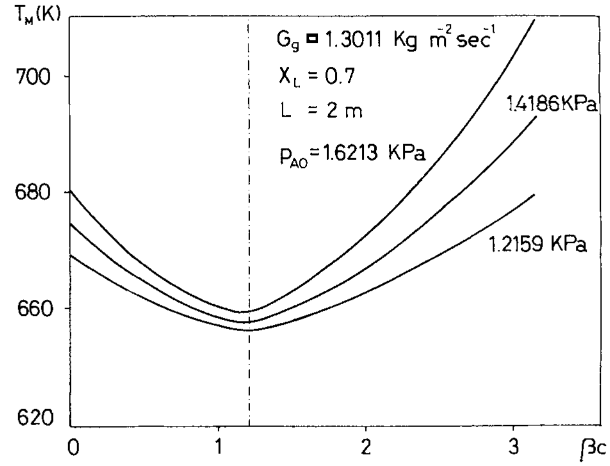


**Figure 5. $T_M$ vs. $\beta c$ curves at different inlet partial pressures.**

tions. It may be convenient at this point to introduce a dimensionless heat-loss coolant parameter, $\beta c = DL$. From the definition of $D$, $\beta c$ can be shown to be inversely proportional to the coolant flow rate, and can be substituted for $Wc^{-1}$ in the abscissa axis of Figure 2. On doing this, as in Figure 3, a first inspection reveals that the $T_M$ curves corresponding to different reactor lengths present their minima, approximately, at a unique value of the abscissa. A similar behavior is found when the effect of changes in other operation variables is analyzed. This is illustrated in Figures 4 and 5, where $T_M$ vs. $\beta c$ curves are drawn for different values of the reactants' flow rate and the inlet partial pressure, respectively.

A second aspect of interest is that the $\beta c$ values corresponding to the minima of the $T_M$ curves are practically coincident in the cases of Figures 3 to 5, which have the same outlet conversion ($x_L = 0.7$) in common. Consequently, the optimization problem could be reformulated as follows: find the optimum value of the coolant flow rate, $Wc_{\text{opt}}$ (or its correspondent, $\beta c_{\text{opt}}$) which for a given conversion, $x_L$, leads to a minimum for the maximum temperature ($T_{M_m}$). In other words, the problem can be reduced to finding $\beta c_{\text{opt}}$ as a function of $x_L$.

In the previous section it was stated that for prespecified inlet conditions, the ideal isothermal operation is the one which leads to the thermal profile with minimum $T_M$. Therefore, it looks reasonable to investigate whether the coolant parameters, $\beta c_i$, correspondent to the equivalent isothermal operation, is an adequate approximation to the optimal cooling design defined above (equivalent isothermal operation can be defined as the one which, starting from the same reactant mass flow rate, leads to the same conversion, $x_L$, in the same total length, $L$).

Assuming the previous statement is correct, the following expression can be derived from Eq. 7:

$$\beta c_{\text{opt}} \simeq \beta c_i = \ln\left[\frac{1}{1 - x_L}\right] \tag{8}$$

The abscissa indicated with a dotted line in Figures 3 to 5, corresponds to the isothermal value, $\beta c_i = 1.204$, which was calculated from Eq. 8 where $x_L = 0.7$. It can be seen, as expected, that this simple expression gives a good approximation of the locus of the minimums of $T_M$. The same behavior was found for different values of $x_L$, as shown in Figure 6, where the minima of

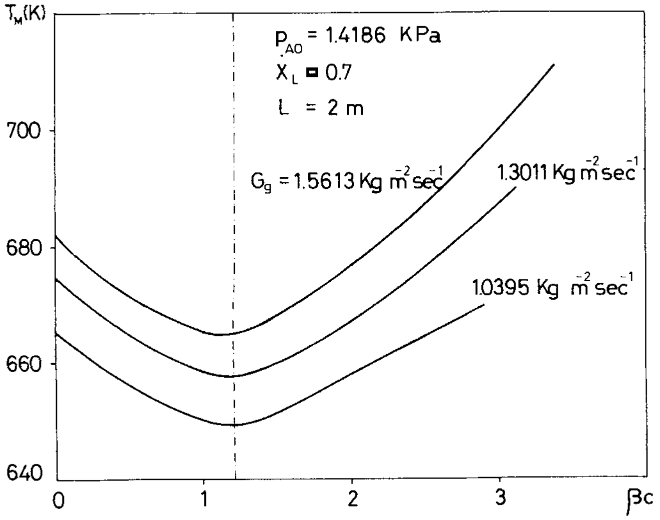


**Figure 4. $T_M$ vs. $\beta c$ curves at different specific mass flow rates.**

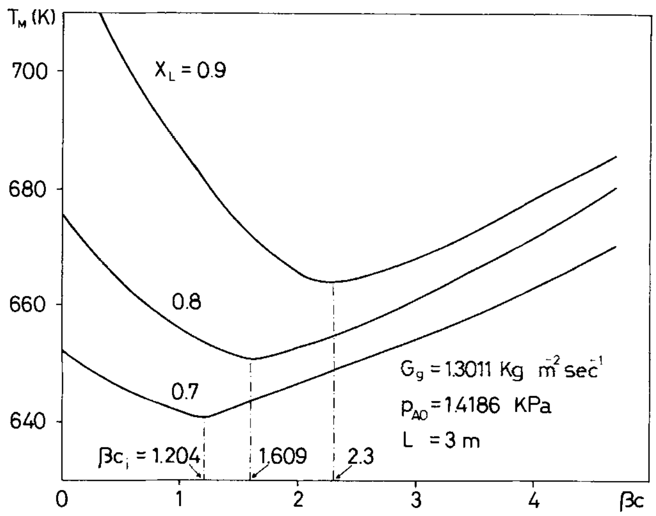


**Figure 6. $T_M$ vs. $\beta c$ curves at different outlet conversion levels.**

the $T_M$ vs. $\beta c$ curves are practically coincident with the values of $\beta c_i$.

Therefore, if the cooling section is designed in the proposed way (cocurrent, $\beta c = \beta c_i$), the unit could be operated in conditions very near to those corresponding to the minimum $T_M$. It is also important to recall that in these conditions the values of $S^*$ will be only slightly higher than the corresponding $S^*_m$.

As a sequel to a previous paper (Borio et al., 1989) where the advantages of the cocurrent configurations were demonstrated, the analytical expressions introduced here permit, in a simple and direct way, the calculation of the optimal coolant flow rate. The implementation of the proposed cooling strategy in industrial units where countercurrent or perfectly mixed cooling schemes are in current use, would lead to a significant improvement in the safety of the reactor operation.

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## Notation

$a = E/R$
$A = (\rho_b\, P\, M\, p_{B_o})/(G_g)$
$B = (\rho_b(-\Delta H) p_{B_o})/(G_g\, c_{p_g})$
$C = (4U)/(d_t\, G_g\, c_{p_g})$
$c_p$ = specific heat, KJ · Kg$^{-1}$ · K$^{-1}$
$d$ = diameter, m
$D = (\pi\, d_t\, t_n\, U)/(Wc\, c_{p_c})$
$E$ = activation energy, KJ · Kmol$^{-1}$
$G$ = specific mass flow rate, Kg · m$^{-2}$ · s$^{-1}$
$k_\infty$ = preexponential factor, Kmol · s$^{-1}$ · Kgcat$^{-1}$ · KPa$^{-2}$
$L$ = total reactor length, m
$M$ = molecular weight of gaseous mixture, Kg · Kmol$^{-1}$
$p$ = partial pressure, KPa
$P$ = total pressure, KPa
$R$ = universal gas constant, KJ · Kmol$^{-1}$ · K$^{-1}$
$S^*$ = absolute extreme (max or min) of $\partial T(z)/\partial Tc_j$ curves, K/K
$t_n$ = number of reactor tubes
$T$ = temperature inside reactor tubes, K
$Tc$ = temperature of cooling fluid, K
$U$ = overall heat transfer coefficient, KW · m$^{-2}$ · K$^{-1}$
$Wc$ = cooling mass flow rate, Kg · s$^{-1}$
$x$ = conversion
$z$ = axial coordinate, m

### *Greek letters*

$\beta c$ = dimensionless cooling heat-loss parameter
$\Delta H$ = heat of reaction, KJ · Kmol$^{-1}$
$\rho$ = density, Kg · m$^{-3}$

### *Subscripts*

$A$ = O-xylene
$b$ = bulk
$B$ = second component
$c$ = cooling medium
$g$ = gas
$i$ = isothermal operation
$j$ = at inlet axial position
$L$ = at axial position, $z = L$
$m$ = minimum
$M$ = at maximum temperature axial position
$o$ = at axial position, $z = 0$
opt = optimal
$t$ = tube

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