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F. Logist, P.M. Van Erdeghe and J.F. Van Impe 2009. Efficient deterministic multiple objective optimal control of (bio)chemical processes. Chemical Engineering Science, 64, 2527-2538.

The journal and the original published paper can be found at:

<http://www.sciencedirect.com/science/journal/00092509/>

<http://dx.doi.org/10.1016/j.ces.2011.06.018>

The corresponding author can be contacted for additional info.

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Efficient deterministic multiple objective optimal control of (bio)chemical processes

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Abstract

In practical optimal control problems multiple and conflicting objectives are often present, giving rise to a set of Pareto optimal solutions. Although combining the different objectives into a convex weighted sum and varying the weights is the most common approach to generate the Pareto front (when deterministic optimisation routines are exploited), it suffers from several intrinsic drawbacks. A uniform variation of the weights does not necessarily lead to an even spread on the Pareto front, and points in non-convex parts of the Pareto front cannot be obtained (Das and Dennis, 1997). Therefore, this paper investigates alternative approaches based on novel methods as Normal Boundary Intersection (Das and Dennis, 1998) and Normalised Normal Constraint (Messac et al., 2003; Messac and Mattson, 2004) to mitigate these drawbacks. The resulting multiple objective optimal control procedures are successfully used in (i) the design of a chemical reactor with conflicting conversion and energy costs, and (ii) the control of a bioreactor with a conflict between yield and productivity.

Key words: bioreactors, chemical reactors, control, dynamic optimisation, multiple objectives, deterministic optimisation routines

Postprint of manuscript accepted for Chemical Engineering Science

1 Introduction

In practice, optimising the design and operation of (bio)chemical processes often gives rise to optimisation problems with different and conflicting objectives (Bhaskar et al., 2000; Sendin et al., 2006). Typically, these *multiple objective optimisation* (MOO) problems produce a set of optimal solutions (or the *Pareto set*) instead of one sole. The designer will then select one solution from this palette of equally valid solutions.

The research on scalar MOO problems has attracted much attention over the years (see, e.g., the books by Miettinen (1999) and Deb (2001)). Solution methods for generating the Pareto front are broadly classified in two categories (see, e.g., the review by Marler and Arora (2004)). A first class transforms the MOO problem into a series of single objective optimisation problems. By varying the parameters of the method involved, often a representation of the Pareto set is obtained. This class includes the classic convex *Weighted Sum* (WS) of the different objectives, but also encompasses novel methods as *Normal Boundary Intersection* (NBI) (Das and Dennis, 1998), or *Normalised Normal Constraint* (NNC) (Messac and Mattson, 2004). The second class involves population based stochastic methods, e.g., *genetic algorithms* (Srinivas and Deb, 1995; Deb et al., 2002; Konak et al., 2006) and *particle swarm optimisation* (Coello et al., 2004), which have been found to be able to generate the Pareto set directly from the multiple objective formulation.

However, much less effort is spent on *multiple objective optimal control* (MOOC) problems (i.e., when an infinite dimensional optimal control profile has to

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be found for a model described by differential equations (ODEs)). Typical (bio)chemical examples are fermentation and polymerisation processes. Jadot et al. (1998) have studied optimal feeding strategies for a fed-batch bioreactor with a yield - productivity conflict. Trelea et al. (2004) have computed optimal temperature and pressure evolutions for a beer brewing process, which minimise the fermentation time, while also minimising the deviations from certain aroma target values. Optimal feeding profiles for a semi-batch epoxy polymerisation process have been reported by Mitra et al. (2004) in order to produce a polymer of maximum molecular weight in minimum time. In Logist et al. (2008a, 2009) optimal steady-state jacket fluid temperature profiles have been derived for a conceptual tubular reactor with a trade-off between conversion and energy objectives. Alternatively, Agrawal et al. (2007) have obtained optimal steady-state temperatures for the different jackets along an industrial tubular LDPE reactor in view of a maximisation of monomer conversion and a minimisation of side products.

The multiple objective approaches employed to tackle these (bio)chemical MOOC problems are most often (i) weighted sum approaches in which for a grid of different weights optimal control problems are solved with deterministic optimisation routines (Muske and Peyton Jones, 2006; Logist et al., 2007), or (ii) stochastic genetic algorithms in which a population of solutions is updated based on repeated cost computations (and, hence, model simulations) in order to evolve gradually to the Pareto set (Sarkar and Modak, 2004, 2005). Unfortunately, both approaches exhibit certain restrictions. For the weighted sum it is known that an equal distribution of weights does not necessarily lead to an even spread along the Pareto front, and that points in a non-convex part of the Pareto front cannot be obtained (Das and Dennis, 1997). However, recent

techniques as NBI and NNC have been found to mitigate these disadvantages for scalar MOO problems, while still allowing the exploitation of deterministic solvers. Stochastic approaches on the other hand have been quite successful over the last decades (Bhaskar et al., 2000). However, these routines (*i*) may become time consuming due to the repeated model simulations required, (*ii*) may require the proper selection of algorithmic parameters (e.g., population size), (*iii*) are less suited to incorporate constraints exactly, and (*iv*) are limited to rather low dimensional search spaces (due to their more systematic exploration of these spaces). This last aspect restricts the possible control parameterisations to either (*i*) analytical parameterisations based on expressions derived from the necessary conditions of optimality, or (*ii*) coarse piecewise polynomial approximations (e.g., constant or linear functions). Nevertheless, despite the absence of rigorous proofs these stochastic techniques are generally regarded as global optimisation routines (in contrast to deterministic procedures which ensure most often only local optimality).

Therefore, the aim of this paper is to incorporate NBI and NNC (instead of WS) in a deterministic multiple shooting optimal control approach. The modifications allow to efficiently use a fine control discretisation and to flexibly incorporate constraints, while ensuring an equal distribution along the possibly non-convex Pareto front in a limited computation time. Examples related to a tubular chemical reactor with conflicting conversion and energy objectives, and a fed-batch bioreactor with a productivity - yield conflict will be studied. The organisation of the paper is as follows. Section 2 mathematically formulates an MOOC problem, and briefly reviews typical aspects and methods for MOO. Section 3 introduces the case studies, while Section 4 presents the results. Section 5 finally summarises the main conclusions.

2 Multiple-objective optimal control

2.1 Mathematical formulation

An multiple objective optimal control problem can be formulated as follows:

$$\text{minimise } \{J_1(\mathbf{u}(\xi), \xi_f), \dots, J_m(\mathbf{u}(\xi), \xi_f)\} \quad (1)$$

subject to:

$$\frac{d\mathbf{x}}{d\xi} = \mathbf{f}(\mathbf{x}(\xi), \mathbf{u}(\xi), \xi) \quad (2)$$

$$\mathbf{0} = \mathbf{b}_i(\mathbf{x}(0)) \quad (3)$$

$$\mathbf{0} = \mathbf{b}_t(\mathbf{x}(\xi_f)) \quad (4)$$

$$\mathbf{0} \geq \mathbf{c}_p(\mathbf{x}(\xi), \mathbf{u}(\xi), \xi) \quad (5)$$

$$\mathbf{0} \geq \mathbf{c}_t(\mathbf{x}(\xi_f), \mathbf{u}(\xi_f), \xi_f) \quad (6)$$

with $\mathbf{x}$ and $\mathbf{u}$ the state and control variables. The vector $\mathbf{f}$ represents the dynamic system equations (on the interval $[0, \xi_f]$) with consistent initial and terminal boundary conditions given by the vectors $\mathbf{b}_i$ and $\mathbf{b}_t$. The vectors $\mathbf{c}_p$ and $\mathbf{c}_t$ indicate respectively path and terminal inequality constraints on the states, the controls and/or the independent variable ξ . Each individual cost function can be of the following type:

$$J_i = \underbrace{h_i(\mathbf{x}(\xi_f), \xi_f)}_{\text{Terminal cost}} + \underbrace{\int_0^{\xi_f} g_i(\mathbf{x}(\xi), \mathbf{u}(\xi)) d\xi}_{\text{Integral cost}}. \quad (7)$$

Let $\mathcal{U}$ be the feasible region, i.e., the set of all admissible controls $[\mathbf{u}(\xi), \xi_f]$, which induce admissible state trajectories $\mathbf{x}(\xi)$. Linking each element from $\mathcal{U}$ to the corresponding cost vector $\mathbf{J}(\mathbf{u}, \xi_f) = [J_1(\mathbf{u}, \xi_f), \dots, J_m(\mathbf{u}, \xi_f)]^T$ yields the set of feasible cost vectors $\mathcal{J}$.

2.2 Multiple objective optimisation: concepts and methods

Contrary to single objective optimisation, typically no single global solution exists in multiple objective optimisation. Therefore, it is necessary to determine a set of points that all fit a predetermined optimality definition, which is most often the concept of *Pareto optimality*.

Definition: A control $[\mathbf{u}^*, \xi_f^*] \in \mathcal{U}$, is Pareto optimal iff there does not exist another control $[\mathbf{u}, \xi_f] \in \mathcal{U}$, such that $\mathbf{J}(\mathbf{u}, \xi_f) \leq \mathbf{J}(\mathbf{u}^*, \xi_f^*)$ and $J_i(\mathbf{u}, \xi_f) < J_i(\mathbf{u}^*, \xi_f^*)$ for at least one cost.¹

In other words, a control is Pareto optimal if there exists no other control that improves at least one objective function without worsening another.

2.2.1 Weighted Sum

The most often employed deterministic strategy for an MOOC problem is to reformulate it as a single objective optimal control problem with a convex weighted sum of the different objectives:

$$\min_{\mathbf{u}(\xi), \xi_f} J_{tot} = \sum_{i=1}^m w_i J_i \quad \text{with} \quad w_i \geq 0 \quad \text{and} \quad \sum_{i=1}^m w_i = 1 \quad (8)$$

subject to:

Equations (2) to (6).

A geometric interpretation in the cost space is depicted in Figure 1a. For illustrative reasons, a bi-objective problem is depicted and the individual costs

¹ The comparison between vectors has to be interpreted componentwise.

have been normalised. Here, a normalised cost is defined as:

$$\overline{J}_i = (J_i(\mathbf{u}, \xi_f) - J_i(\mathbf{u}_i^*, \xi_{f,i}^*)) / (J_i^\diamond - J_i(\mathbf{u}_i^*, \xi_{f,i}^*)) \quad (9)$$

with $[\mathbf{u}_i^*, \xi_{f,i}^*]$ the individual minimiser of the i -th objective J_i and $J_i^\diamond$ the maximum value of the i -th objective for the set of all individual minimisers:

$$J_i^\diamond = \max\{J_i(\mathbf{u}_k^*, \xi_{f,k}^*) | k = 1 \dots m\}. \quad (10)$$

A certain set of weights (i.e., $w_1 = 1 - w$ and $w_2 = w$) corresponds to a certain angle of the line L (i.e., $\theta + \pi/2$ with $\theta = \pi/2 - \arctan(w/(1 - w))$). Minimising the convex sum is equivalent to shifting the line L parallelly from the origin, until it touches the boundary of the (normalised) feasible cost space $\overline{\mathcal{J}}$. In the current case, this results in the Pareto optimal point A. Varying the weights leads to different slopes, and consequently different Pareto points. As can be deduced, points between B and C, i.e., points in the non-convex part of the Pareto set, cannot be obtained since the line BC cannot be crossed by the parallel lines without intersecting the boundary of the feasible region elsewhere. In addition, it can easily be imagined that a uniform distribution of the weights not necessarily yields an even spread on the Pareto set.

2.2.2 Normal Boundary Intersection

NBI tackles the MOO from a geometrically intuitive viewpoint. It first builds a plane in the cost space which contains all convex combinations of the individual minima, i.e., the *convex hull of individual minima* (CHIM), and then constructs (*quasi*-)normal lines to this plane. The rationale behind the method is that the intersection between the (quasi-)normal from any point $\mathbf{J}_p$ on the

CHIM, and the boundary of the feasible cost space closest to the origin is expected to be Pareto optimal. Hereto, the multiple objective problem is reformulated as to maximise the distance λ from a point $\mathbf{J}_p$ on the CHIM along the quasi-normal through this point, without violating the original constraints. Technically, this requirement of lying on the quasi-normal introduces additional equality constraints. By selecting the points on the CHIM with an equal spread, also an equal spread on the Pareto frontier in the objective space is obtained. Mathematically, NBI is formulated as follows:

$$\max_{\mathbf{u}(\xi), \xi_f, \lambda} \lambda \quad (11)$$

subject to:

$$\begin{array}{l} \text{Equations (2) to (6)} \\ \Phi \mathbf{w} - \lambda \Phi \mathbf{e} = \mathbf{J}(\mathbf{u}, \xi_f) - \mathbf{J}^* \end{array} \quad (12)$$

Here, Φ is the pay-off matrix in which the i -th column is $\mathbf{J}(\mathbf{u}_i^*, \xi_{f,i}^*) - \mathbf{J}^*$, with $[\mathbf{u}_i^*, \xi_{f,i}^*]$ being the minimiser of the i -th objective J_i and $\mathbf{J}^*$ being the utopia point, which contains the minima of the individual objectives $J_i(\mathbf{u}_i^*, \xi_{f,i}^*)$. $\mathbf{w}$ is a vector of weights such that $\sum_{i=1}^m w_i = 1$ with $w_i \geq 0$, and $\mathbf{e}$ is a vector containing all ones. Now, $\Phi \mathbf{w}$ describes a point in the CHIM and $-\Phi \mathbf{e}$ defines the (quasi-)normal to the CHIM pointing towards the origin.

A geometric interpretation of NBI for a bi-objective case is presented in Figure 1b. The CHIM is the line connecting the (normalised) individual minima $\bar{J}_1 = 1$ and $\bar{J}_2 = 1$. Points $\bar{\mathbf{J}}_p$ are uniformly selected on this line (by the use of weight vectors $\mathbf{w} = [1 - w, w]^T$ in which w is selected uniformly from 0 to 1). Each time the quasi-normal is constructed and the intersection with

the boundary of the feasible cost region $\overline{\mathcal{J}}$ closest to the origin is sought. This feature is represented by the arrows. It should be noted that the equality constraints (i.e., Equation (12)) imposing the requirement to be part of the (quasi-)normal further restrict the feasible region. This restriction is illustrated by the darker colour (of the area beside the arrows) compared to the colour in Figure 1a. As can be seen, Pareto optimal points in the non-convex parts can readily be obtained.

Advantages are the equal distribution of points along the Pareto set. However, although this method is able to detect Pareto solutions in non-convex parts of the Pareto frontier, it may also return non-Pareto optimal or dominated points, and it may overlook some Pareto optimal points for more than two objectives.

2.2.3 Normalised Normal Constraint

NNC employs similar ideas as NBI, but combines them with features of the ε -constraint method (Haimes et al., 1971). This ε -constraint method minimises the single most important objective function J_k , while the $m - 1$ other objective functions are added as inequality constraints of the form $J_i \leq \varepsilon_i$. These inequalities can be interpreted as hyperplanes reducing the feasible criterion space. As in NBI, in NNC first a plane (called here, the *utopia hyperplane*) is constructed through all individual minima (which have been normalised in this case), and second, equally distributed points $\overline{\mathbf{J}}_p$ in this plane are determined by consistently varying the weights. NBI requires the maximisation of the distance along the quasi-normal through points $\overline{\mathbf{J}}_p$ on the CHIM, and, hence, reduces the feasible objective space by equality constraints. In contrast, simi-

larly to the ε -constraint method, NNC minimises a selected objective $\bar{J}_k$, given the original constraints, and while additionally reducing the feasible space by adding $m - 1$ hyperplanes through the selected point $\bar{\mathbf{J}}_p$ in the utopia plane. These hyperplanes are chosen perpendicular to each of the $m - 1$ *utopia plane vectors*, which join the individual minimum $\bar{\mathbf{J}}(\mathbf{u}_k^*, \xi_{f,k}^*)$ corresponding to the selected objective $\bar{J}_k$, with all other individual minima $\bar{\mathbf{J}}(\mathbf{u}_i^*, \xi_{f,i}^*)$ (and, thus, span the utopia hyperplane itself). This approach leads to an additional set of inequality, instead of equality constraints. Mathematically, this yields the following formulation:

$$\min_{\mathbf{u}(\xi), \xi_f} \bar{J}_k \quad (13)$$

subject to:

$$\begin{array}{c} \text{Equations (2) to (6)} \\ (\bar{\mathbf{J}}(\mathbf{u}_k^*, \xi_{f,k}^*) - \bar{\mathbf{J}}(\mathbf{u}_i^*, \xi_{f,i}^*))^T (\bar{\mathbf{J}}(\mathbf{u}, \xi_f) - \bar{\mathbf{J}}_p) \leq 0 \quad i = 1 \dots m, i \neq k. \end{array} \quad (14)$$

Here, the points $\bar{\mathbf{J}}_p$ are selected in a similar way as in NBI, i.e., by using (i) a vector of weights $\mathbf{w}$ such that $\sum_{i=1}^m w_i = 1$ with $w_i \geq 0$ and (ii) the (normalised) pay-off matrix.

The geometric interpretation of NNC (see Figure 1c) is similar to the one of NBI. The CHIM is now replaced by the utopia hyperplane (here, the utopia line). One perpendicular hyperplane (here, the line normal to the vector joining the individual minima $\bar{J}_1$ and $\bar{J}_2$) is required to reduce the feasible space for minimising the selected objective (here, $\bar{J}_1$). However, as inequality constraints (Equations (14)) are imposed, only part of the original feasible cost region becomes now prohibited territory (indicated by the darker colour). Again,

a uniform spread on the utopia plane of points $\overline{\mathbf{J}}_p$ (by the use of weight vectors $\mathbf{w} = [1 - w, w]^T$ in which w is selected uniformly from 0 to 1), results in an even spread along a possibly non-convex Pareto frontier. Hence, this approach exhibits the same advantages as NBI, but it also suffers from similar drawbacks.

3 Case studies

The different MOOC techniques are illustrated for one chemical application, i.e., a jacketed tubular chemical reactor, and one biochemical application, i.e., a fed-batch bioreactor. For each application two case studies are elaborated. The choice of these case studies has mainly been driven by the existence of analytical (and thus exact) solutions to which any purely numerical result (e.g., with a fine piecewise constant control parameterisation) can easily be compared.

3.1 Tubular chemical reactor

The investigated reactor is a jacketed tubular reactor with a fixed length L [m] as studied by Smets et al. (2002); Logist et al. (2008b, 2009). The reactor operates under steady-state conditions and inside an exothermic irreversible first-order reaction takes place. The aim is to design an optimal profile along the reactor for the jacket fluid temperature T_w [K] in view of conflicting conversion and energy costs.

3.1.1 Reactor model

For the reactor model (i) a constant density of the reaction mixture, (ii) perfect radial mixing and (iii) an Arrhenius dependence of the reaction rate on the temperature are assumed. However, based on the absence (or presence) of dispersive phenomena, either a Plug Flow Reactor (PFR), or a Dispersive Flow Reactor (DFR) model has to be employed.

Assuming plug flow yields the following PFR model equations:

$$\frac{dx_1}{dz} = \frac{\alpha}{v}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} \quad (15)$$

$$\frac{dx_2}{dz} = \frac{\alpha\delta}{v}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} + \frac{\beta}{v}(u - x_2) \quad (16)$$

and boundary conditions at the inlet:

$$x_1(0) = 0 \quad (17)$$

$$x_2(0) = 0. \quad (18)$$

The presence of dispersion, however, introduces second-order terms and yields the following DFR model equations:

$$D_C \frac{d^2 x_1}{dz^2} = +v \frac{dx_1}{dz} - \alpha(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} \quad (19)$$

$$D_T \frac{d^2 x_2}{dz^2} = +v \frac{dx_2}{dz} - \alpha\delta(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}} - \beta(u - x_2) \quad (20)$$

and split Danckwerts boundary conditions (Danckwerts, 1953):

$$D_C \frac{dx_1}{dz}(0) = vx_1(0) \quad \text{and} \quad \frac{dx_1}{dz}(L) = 0 \quad (21)$$

$$D_T \frac{dx_2}{dz}(0) = vx_2(0) \quad \text{and} \quad \frac{dx_2}{dz}(L) = 0. \quad (22)$$

Here, $x_1 = (C_F - C)/C_F$ [-] is the dimensionless reactant concentration C [mol/L], $x_2 = (T - T_F)/T_F$ [-], the dimensionless reactor temperature T [K], and $u = (T_w - T_F)/T_F$ [-], the dimensionless jacket temperature T_w [K]. C_F [mol/L] and T_F [K] denote the reactant concentration and temperature of the feed stream. D_C [m²/s] and D_T [m²/s] are the mass and energy dispersion coefficients. v [m/s] represents the fluid velocity. The constants α , β , γ , and δ are defined as follows:

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

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. The exact parameter values are provided in Table 1.

Since the DFR model (Equations (19) to (22)) does not fit into the general MOOC formulation (Equations (2) to (6)), the gradients $dx_1/dz = x_3$ [1/m] and $dx_2/dz = x_4$ [1/m] have to be introduced as additional state variables in order to convert the two second-order ODEs to four first-order ODEs.

3.1.2 Objectives

As the jacket temperature T_w is in practice often used to control the reactor, this variable is selected as the control $u(z)$. Note that the spatial coordinate z [m] is now the independent variable. The aim is to derive a jacket fluid temperature profile that minimises the reactant concentration at the outlet (i.e., maximises conversion):

$$J_1 = C_F(1 - x_1(L)) \quad (23)$$

while minimising the terminal heat loss:

$$J_2 = \frac{T_F^2 x_2^2(L)}{K}. \quad (24)$$

with K [-] a scaling factor (see, Smets et al. (2002)). Clearly, these are conflicting goals since high temperatures favour conversion.

3.1.3 Constraints

To avoid hazardous situations explicit bounds are added on the reactor and the jacket temperature:

$$x_{2,min} \leq x_2(z) \leq x_{2,max} \quad (25)$$

$$u_{min} \leq u(z) \leq u_{max} \quad (26)$$

with $x_{2,min} = (T_{min} - T_F)/T_F$, $x_{2,max} = (T_{max} - T_F)/T_F$, $u_{min} = (T_{w,min} - T_F)/T_F$, and $u_{max} = (T_{w,max} - T_F)/T_F$.

3.1.4 Case study specifications

Two cases are studied for the tubular reactor, i.e., Case I, employing the PFR model, and Case II based on the DFR model. Mathematically, both cases give rise to nonlinear MOOC problems with control and state inequality path constraints. With respect to the underlying model, Case I involves only two ODEs with specified initial conditions (i.e., an initial value problem), while Case II gives rise to four ODEs and split boundary conditions (i.e., a boundary value problem). Table 2 concisely summarises both cases.

3.2 Fed-batch bioreactor

The studied bioreactor is based on the fed-batch lysine fermentation process investigated by Ohno et al. (1976). The aim is to determine an optimal feeding profile and batch length with respect to conflicting yield and productivity objectives.

3.2.1 Reactor model

Assuming perfect mixing and no product degradation yields the following model equations:

$$\frac{dx_1}{dt} = +\mu x_1 \quad (27)$$

$$\frac{dx_2}{dt} = -\sigma x_1 + u C_{s,F} \quad (28)$$

$$\frac{dx_3}{dt} = +\pi x_1 \quad (29)$$

$$\frac{dx_4}{dt} = +u \quad (30)$$

with as states variables x_1 [g], the biomass, x_2 [g], the substrate, x_3 [g], the product (lysine), and x_4 [L] the fermenter volume. The control u [L/h] is the volumetric rate of the feed stream, which contains a limiting substrate concentration $C_{s,F}$ of 2.8 g/L. Note that the time t [h] is now the independent variable in the ODEs. The specific rates for growth μ [1/h], substrate consumption σ [g/gh], and production π [g/gh] are given as:

$$\mu = 0.125 C_s \quad (31)$$

$$\sigma = \mu / 0.135 \quad (32)$$

$$\pi = -384 \mu^2 + 134 \mu \quad (33)$$

with C_s [g/L] the substrate concentration. The initial conditions are specified as:

$$x_1(0) = 0.1 \text{ g} \quad (34)$$

$$x_2(0) = 14 \text{ g} \quad (35)$$

$$x_3(0) = 0 \text{ g} \quad (36)$$

$$x_4(0) = 5 \text{ L} \quad (37)$$

3.2.2 Objectives

As the process is operated in fed-batch mode with an unspecified duration, both the feed rate, i.e., the control $u(t)$ and the final time t_f have to be determined. The aim is to derive a feeding strategy which maximises the productivity, i.e., the ratio between the product formed and the process duration:

$$J_p = \frac{x_3(t_f)}{t_f} \quad (38)$$

while maximising the yield. However, several interpretations for the yield exist. For instance, Sarkar and Modak (2005), who studied the same fermentation process, computed it as the ratio of the amount of product formed and the amount of substrate consumed. Here, the total amount of consumed substrate equals the sum of the substrate initially present in the tank and the mass of substrate added during operation minus the substrate remaining at the operation end. Since in the current case, the substrate concentration in the tank at the start $C_s(0) = x_2(0)/x_4(0)$ is identical to the substrate concentration in the feed $C_{s,F}$, the yield can be expressed as:

$$\begin{aligned} J_y^a &= \frac{x_3(t_f)}{(x_4(0)C_s(0) + (x_4(t_f) - x_4(0))C_{s,F} - x_2(t_f))} \\ &= \frac{x_3(t_f)}{(x_4(t_f)C_{s,F} - x_2(t_f))}. \end{aligned} \quad (39)$$

Alternatively, the yield can be defined as the mass of product over the mass of substrate added:

$$J_y^b = \frac{x_3(t_f)}{(x_4(0)C_s(0) + (x_4(t_f) - x_4(0))C_{s,F}} = \frac{x_3(t_f)}{(x_4(t_f)C_{s,F})}. \quad (40)$$

In the current study, two yield interpretations will be tested: (i) Equation (39), which is based the substrate consumed and has been employed by Sarkar and

Modak (2005), and (ii) one which only accounts for the substrate added during the process (and, thus neglects the 14 g of substrate initially present):

$$J_y^c = \frac{x_3(t_f)}{(x_4(t_f) - x_4(0))C_{s,F}}. \quad (41)$$

Equation (39) has been selected as it allows a comparison to the results reported by Sarkar and Modak (2005). Despite its slightly artificial character, Equation (41) has been adopted because it gives rise to (numerically) interesting phenomena.

To cast these maximisation problems into a minimisation framework (Equations (1) to (6)) the cost functions are defined as the negative productivity and yield: $J_1 = -J_p$ and $J_2 = -J_y^a$ (or $J_2 = -J_y^c$, respectively).

3.2.3 Constraints

For practical reasons constraints are imposed on the volume, the feed rate and the operation time.

$$5 \text{ L} \leq x_4(t) \leq 20 \text{ L} \quad (42)$$

$$0 \text{ L/h} \leq u(t) \leq 2 \text{ L/h} \quad (43)$$

$$20 \text{ h} \leq t_f \leq 40 \text{ h} \quad (44)$$

In addition, to avoid indefinite cost values when the initial amount of substrate is neglected in the yield, a lower bound of 20 g is imposed on the amount of substrate added through feeding after time $t=0$ s:

$$20 \text{ g} \leq (x_4(t_f) - x_4(0))C_{s,F}. \quad (45)$$

3.2.4 Case study specifications

Also for the bioreactor two cases are investigated, i.e., Case III (with objectives J_p & J_y^a), which accounts for the consumed amount of substrate, and Case IV (with objectives J_p & J_y^c), which takes the substrate fed into account (but neglects the initial amount) and adds a lower bound on the amount fed during the operation. From a mathematical viewpoint, both cases involve a nonlinear free end time MOOC problem described by 4 ODEs with given initial values. Inequality path constraints are specified for the control and one state, while bounds are imposed on the end time. In Case IV, the additional lower bound on the amount fed provides an additional terminal inequality constraint. The equations for Cases III and IV are also summarised in Table 2.

4 Results

The software package MUSCOD-II (Leineweber et al., 2003a,b), which tackles optimal control problems by a deterministic multiple shooting approach (Bock and Plitt, 1984), is employed to generate the Pareto front for each of the four cases. Each time WS, NBI and NNC are implemented, and a uniform grid with 11 points is selected for the parameter w (i.e., $w \in [0 : 0.1 : 1]$). Hereby, the fractions $1 - w$ and w are linked to the first and second objective, respectively. The resulting Pareto sets are compared for two types of control parameterisations. First, a piecewise constant control parameterisation (PWC) (with 50 pieces of equal length) is used. Second, an analytical control parameterisation (AP) (Srinivasan et al., 2003) is employed, which is based on (i) analytical expressions obtained from the necessary conditions of optimality (NCO) and (ii) the optimal sequence of arcs identified from the PWC results. Consequently, this AP has mainly the switching positions as degrees of freedom and yields exact optimal solutions to which the PWC results can be compared.

It should, however, be noted that possibly not all arcs (e.g., very short bang-bang type of arcs required to enter, e.g., a path constrained arc) may be identified from a piecewise constant parameterisation. Hereto, it is valuable to analyse (i) the degrees of freedom of the identified arc sequence and (ii) the profile and pointwise constraints originating from the necessary conditions of optimality (NCO), (see also Srinivasan and Bonvin (2007) for a more detailed discussion). However, in the same paper, it is also mentioned that neglecting these short arcs is in general not harmful for practical implementations.

For the four cases, the set of possible optimal control arcs and their analytical expressions is provided in Table 2. For completeness, the values for the obtained individual minima are provided in Table 3. Since NBI and NNC yield in the current investigation identical Pareto sets for all four cases studied, only one Pareto front for both methods is depicted due to space restrictions. As in addition hardly any differences have been observed between the PWC and the AP results (with respect to Pareto sets and optimal profiles) all displayed plots refer to AP results, except that the optimal PWC profiles have been added to illustrate the similarities between the two parameterisations. The possibility of missing short arcs of bang-bang type has been investigated also via optimising AP sequences with additional max and/or min arcs. However, for none of the tested cases, the addition of arcs did yield an improvement (since the length of the additional arcs was always reduced to zero).

4.1 Tubular chemical reactor

4.1.1 Case I

The resulting Pareto frontiers for the PFR case are depicted in Figure 2. As expected minimising the reactant outlet concentration and minimising the heat loss are conflicting objectives because lowering one results in an increase of the other. Although all the MOOC approaches capture this feature, large differences in the accuracy of the resulting Pareto sets are visible. Although a uniform grid is used to vary the parameter w in all three MOOC approaches, the results for NBI and NNC clearly exhibit a more uniform spread along the Pareto set than the ones for WS, and, hence, provide a more accurate representation.

The corresponding optimal profiles obtained with NBI are displayed in Figure 3. The first two graphs depict the optimised controls with a PWC and an AP, respectively, while the last two graphs represent the states corresponding to the optimal AP controls. Clearly, the optimal jacket fluid temperature profiles consist of a sequence $u_{max}-u_{min}-u_{path}-u_{min}$, where the total length of the last *min* interval reduces to zero for decreasing w -values. The corresponding temperature profiles exhibit a typical trapezoidal shape of which the decrease shifts towards the outlet. The explanation is that heating the reactor as fast as possible, and maintaining the upper reactor temperature limit of 400 K, stimulates conversion for an exothermic irreversible first-order reaction, whereas cooling the reactor towards the outlet reduces the terminal heat loss and allows to recover energy. The little *min* part in between the *max* and *path* constrained arc is, however, required since the path constrained arc cannot be entered directly without violating the lower bound. The concentration profiles substantiate these observations as decreasing the w -values cause lower outlet concentrations. It should also be noted that the obtained PWC control closely follows the exact AP. Hence, it can be concluded that both parameterisations accurately solve the nonlinear MOOC problem with path constraints and the underlying initial value problem.

4.1.2 Case II

Similar conclusions apply to the DFR case with mass and heat Peclet numbers $Pe_C = vL/D_C$ and $Pe_T = vL/D_T$ equal to 10 (see Figure 4). A uniform grid of weights w results for the WS in a highly skew distribution on the convex Pareto front, while NBI and NNC yield an accurate approximation. Similar to the PFR case, a convex Pareto set is obtained, but the resulting minimal values

are higher for both costs in the current case. This observation is explained by the fact that dispersion or mixing is known to be undesired for an irreversible first-order reaction.

Figure 5 displays the optimal PWC and AP profiles, as well as the state profiles corresponding to the NNC AP results. Again the trapezoidal temperature shape is clearly present for the same reasons as explained above. However, it should be noted that gradients inside the reactor are smoothed due to the mixing. In addition, to satisfy the Danckwerts boundary conditions the inlet values for both states ($C(0) \approx 0.16$ mol/L and $T(0) \approx 360$ K) deviate from the feed values ($C_F = 0.02$ mol/L and $T_F = 340$ K), and zero gradients are encountered at the outlet. Also the optimal sequence of arcs has changed with respect to the PFR case, and consists in the current case of a sequence u_{max} - u_{path} - u_{max} - u_{min} , where the total length of the last two (max and min) intervals reduces to zero for decreasing w -values. The second max part is necessary to induce a negative temperature gradient which is again brought to zero at the outlet by the last min piece. Again, the PWC and AP controls are very similar, despite the more noisy behaviour of the PWC parameterisation on the u_{path} arc. This nervous behaviour is related to the fact that the control (i.e., jacket fluid temperature) influences the reactor temperature not directly, but only via the reactor temperature gradient. In summary, this MOOC problem consisting of an (apparently simple but in practice challenging) boundary value problem and inequality path constraints has been solved accurately.

4.2 Fed-batch bioreactor

4.2.1 Case III

As can be seen in Figure 6, the convex Pareto set for the fed-batch lysine production of Case III illustrates nicely the intrinsic trade-off between yield and productivity. Again, NBI and NNC produce a more balanced Pareto set than WS. The optimal profiles obtained with NNC are displayed in Figure 7. As optimal feeding profiles *max-min-sing-min* type sequences come forward. These types of arc sequences have been reported by, e.g., Van Impe et al. (1994), Van Impe (1998) and Van Impe and Bastin (1998), as generic switching structures for various fermentation processes and cost functions. When only productivity is aimed at (i.e., $w = 0$), the initial *max* part is present in order to stimulate biomass growth, and hence lysine production. However, when the focus shifts towards yield optimisation (i.e., w evolves to one), three phenomena are observed: (i) the *max* piece shortens and vanishes, (ii) the singular profile lowers but lasts longer, and (iii) the total process duration grows to finally reach the maximum value of 40 h. Consequently, more lysine can be produced with the same amount of substrate but at the expense of longer process times.

Sarkar and Modak (2005) have tackled the same MOOC problem using the multiple objective genetic algorithm NSGA-II and an analytical parameterisation approach. The singular arc expression employed by these authors has two parameters and closely approximates the optimal analytical feedback law derived by Modak and Lim (1987). In Figure 6 the extremal points of the Pareto set reported by Sarkar and Modak (2005) are also indicated. As can be

seen, the results provided by NSGA-II, are obtained with the same accuracy when using the current approaches. In addition, the current methods are able to extend the Pareto set presented by Sarkar and Modak (2005) to higher yield and productivity values. The extension on the yield axis is small, while the extension on the productivity axis is more significant. This difference can mainly be attributed to the fact that Sarkar and Modak (2005) have only reported Pareto optimal points corresponding to *min-sing-min* type controls. However, it is seen that for the current case a (relatively short) initial *max* arc is advantageous for productivity, while such arc is not always easily detected by numerical approaches.

4.2.2 Case IV

From a multiple objective perspective is Case IV the most interesting since it exhibits a non-convex Pareto front (see Figure 8). As can be seen, this non-convexity cannot be tackled by the WS (in addition to the non-uniform spread along the Pareto set for points generated by a uniform grid of weights). Clearly, NBI and NNC do not suffer from these weaknesses and are able to provide an accurate representation of this non-convex Pareto set. However, it should be noted that this non-convexity is intrinsic (and is, hence, not related to the local character of the used deterministic optimisation routines) since its presence has been confirmed by an extensive grid search for (approximately) determining the optimal switching positions of the analytical parameterisation.

The optimal profiles obtained with NNC are displayed in Figure 9. A similar evolution as in Case III is present, the *max-min-sing-min* control observed for

low w -values, evolves to a *min-sing-min* control, while the singular feeding rate reduces in height and the fermentation time increases until the maximum admissible value of 40 h is reached (see, e.g., $w = 0.5$ and $w = 1.0$). However, in between these two w -values (see, e.g., $w = 0.7$) the total duration decreases again. Apparently, the gain in productivity by shorter fermentation times outperforms the loss in yield in this region. With respect to the parameterisations used, the PWC parameterisation clearly coincides with the analytical singular control law of the AP. In summary, this nonlinear singular free end time MOOC problem, which gives rise to a non-convex Pareto front, can accurately be solved by both the NBI and NNC based approaches.

4.3 Computational expense

To provide an indication of the computational burden Table 4 depicts the total number of SQP iterations and the total computation time required to generate each time a Pareto front with 11 points. The employed computer has a dual AMD Opteron250 (2.4 GHz) processor and 2 GB RAM, while the integration and optimality tolerances used are 10^{-11} and 10^{-9} , respectively. To enable a fair comparison, identical initial guesses for all (parametric) single objective optimisation problems have been used within one parameterisation class (i.e., PWC and AP). (However, when the result of one parametric optimisation problem is employed to initialise the next one, an additional speed-up in the computation can be expected.)

As can be seen in Table 4, all representations of the Pareto have been generated within a few minutes. In addition to the fact that NBI and NNC generate more accurate Pareto sets than WS, they also give rise to faster computation times.

Apparently, limiting the feasible region by imposing additional constraints is favourable. The little preference for NBI over NNC can be attributed to the fact that in this case the underlying SQP routines deal more easily with equality than inequality constraints.

When comparing the PWC and AP, the former are optimised faster since they, in spite of a larger number of degrees freedom (i.e., 50 compared to 3 or 4 for the AP), give rise to less nonlinear optimisation problems.

For the different cases, the Cases I and III are in general the most easily solved since they only involve an initial value problem. Adding the terminal constraint in Case IV increases the computation time, while the boundary value problem in Case II requires as expected the largest computation time. For the Cases III and IV, which involve a singular arc, the PWC parameterisations require a higher number of SQP iterations due to the shallow minimum compared to Cases I and II, which are determined by active constraints. On the other hand, when the analytical arc expressions are used, the singular MOOC problems, i.e., Cases III and IV, are more easily optimised.

5 Conclusion

In this paper it has been demonstrated that novel scalar multiple objective optimisation (MOO) approaches as Normal Boundary Intersection (NBI) and Normalised Normal Constraint (NNC) can be incorporated in deterministic multiple shooting methods to efficiently solve multiple objective optimal control (MOOC) problems arising in the (bio)chemical industry. It has been shown that intrinsic drawbacks of the classic Weighted Sum approach as (i) the unclear relation between a uniform grid of weights and the spread on the Pareto front, and (ii) the impossibility to obtain points in non-convex parts of the Pareto front, can be mitigated.

Two (bio)chemical applications (i.e., a tubular chemical reactor and a fed-batch bioreactor) have been studied, resulting in four case studies. The MOOC problems in the four cases exhibited several general features, e.g., nonlinear initial as well as boundary value problems, path constraints on the controls and/or states, fixed and free end time, presence and absence of singular arcs, etc. As parameterisation of the control profile both a fine piecewise constant and an analytical parameterisation have successfully been employed. Both parameterisation types have yielded the same Pareto sets and profiles. Hence, this fine piecewise constant parameterisation allows to compute accurate control profiles and, thus, can also be employed for large systems for which analytical control expressions are not readily obtained. Consequently, the approaches presented are not restricted to a small number of parameters (resulting in a coarse control discretisation) as, e.g., stochastic population based multiple objective methods. Moreover, due to the deterministic multiple shooting approach the presented procedures (i) cope more easily and efficiently with

(in)equality constraints and boundary value problems, and (ii) ensure tight tolerances for integration and (local) optimality. In addition, no algorithmic parameters have to be tuned (in contrast to stochastic algorithms) and the required computation times on a standard PC remain very low, i.e., in the order of a few minutes for the entire Pareto set. As the computational features of NNC and NBI are similar, only a very little preference for NBI is given.

In summary, the combination of NBI and NNC with multiple shooting optimal control techniques may pave the way to an efficient and accurate treatment of multiple objective optimal control problems (i) with (bio)chemical processes described by large sets of ordinary differential (and algebraic) equations, and (ii) subject to a number of (in)equality constraints.

6 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.

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Fig. 1. Geometric interpretation in the cost space of methods for solving multiple objective optimisation problems: weighted sum (a), normal boundary intersection (b), and normalised normal constraint (c).

Fig. 2. Tubular chemical reactor Case I: Pareto set generated by the weighted sum (a), and normal boundary intersection / normalised normal constraint (b).

Fig. 3. Tubular chemical reactor Case I: optimal profiles obtained with normal boundary intersection for (i) the control (i.e., the jacket fluid temperature) with a PWC (a) and an AP (b), and (ii) the states, i.e., the concentration (c) and the reactor temperature (d).

Fig. 4. Tubular chemical reactor Case II: Pareto set generated by the weighted sum (a), and normal boundary intersection / normalised normal constraint (b).

Fig. 5. Tubular chemical reactor Case II: optimal profiles obtained with normal boundary intersection for (i) the control (i.e., the jacket fluid temperature) with a PWC (a) and an AP (b), and (ii) the states, i.e., the concentration (c) and the reactor temperature (d).

Fig. 6. Fed-batch bioreactor Case III: Pareto set generated by the weighted sum (a), and normal boundary intersection / normalised normal constraint (b). The solid squares (■) indicate the boundary of the Pareto set reported by Sarkar and Modak (2005).

Table 1

Process parameters for tubular chemical reactor.

Parameter	Value	Parameter	Value
C_F	$= 0.02 \text{ mol/L}$	T_F	$= 340 \text{ K}$
E	$= 47092.5 \text{ J/mol}$	T_{min}	$= 280 \text{ K}$
D_C	$= 0.01 \text{ m}^2/\text{s}$	T_{max}	$= 400 \text{ K}$
D_T	$= 0.01 \text{ m}^2/\text{s}$	$T_{w,min}$	$= 280 \text{ K}$
k_0	$= 10^6 \text{ 1/s}$	$T_{w,max}$	$= 400 \text{ K}$
K	$= 250000$	v	$= 0.1 \text{ m/s}$
L	$= 1 \text{ m}$	β	$= 0.2 \text{ 1/s}$
R	$= 8.3145 \text{ J/mol K}$	δ	$= 0.25$

Fig. 7. Fed-batch bioreactor Case III: optimal profiles obtained with normal boundary intersection for (i) the control (i.e., the feed rate) with a PWC (a) and an AP (b), and (ii) the states, i.e., the biomass (c), the substrate (d), the product (e), and the reactor volume (f).

Fig. 8. Fed-batch bioreactor Case IV: Pareto set generated by the weighted sum (a), and normal boundary intersection / normalised normal constraint (b).

Fig. 9. Fed-batch bioreactor Case IV: optimal profiles obtained with normal boundary intersection for (i) the control (i.e., the feed rate) with a PWC (a) and an AP (b), and (ii) the states, i.e., the biomass (c), the substrate (d), the product (e), and the reactor volume (f).

Table 2

Overview and analytical relations for the different case studies.

	Tubular chemical reactor		Fed-batch bioreactor	
Overview	Case I	Case II	Case III	Case IV
Model	Eqns (15)-(18)	Eqns (19)-(22)	Eqns (27)-(37)	
Objectives	Eqns (23)-(24)		Eqns (38)-(39)	Eqns (38) and (41)
Constraints	Eqns (25)-(26)		Eqns (42)-(44)	Eqns (42)-(45)
Optimal arc expressions	Case I	Case II	Case III	Case IV
At control bounds $u_{min}(\xi)$	$(T_{w,min} - T_F)/T_F$		0 L/h	
$u_{max}(\xi)$	$(T_{w,max} - T_F)/T_F$		2 L/h	
At state bounds $u_{path}(\xi)$	$x_2 - \frac{\alpha\delta}{\beta}(1 - x_1)e^{\frac{\gamma x_2}{1+x_2}}$		0 L/h	
	@ $x_{2,min}$	@ $x_{2,min}$ & $dx_2/d\xi = 0$; or	@ $x_4 = 5$ L or 20 L	@ $x_4 = 5$ L or 20 L; or
	@ $x_{2,max}$	@ $x_{2,max}$ & $dx_2/d\xi = 0$		@ $(x_4(t) - x_4(0))C_{s,F} = 20$ g
Singular (or inside feasible region)	impossible		$\frac{\mu x_1}{0.135(C_{s,F} - x_2/x_4)} \left[1 + \frac{0.135x_4}{\frac{dx_1}{d(x_2/x_4)}} \right]$ with $\frac{dx_1}{d(x_2/x_4)} = -\frac{x_1\mu(\pi''\mu' - \pi'\mu'')}{\mu'(\pi'\mu - \mu'\pi)}$ (Smets et al., 2002) (Logist et al. 2008) (Modak and Lim, 1987)	

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Table 3

Individual minima based on the analytical control parameterisation.

	Individual minimum for J_1		Individual minimum for J_2	
	$J_1(u_1^*, \xi_{f,1}^*)$	$J_2(u_1^*, \xi_{f,1}^*)$	$J_1(u_2^*, \xi_{f,2}^*)$	$J_2(u_2^*, \xi_{f,2}^*)$
Case I	$6.16 \cdot 10^{-5}$	$1.44 \cdot 10^{-2}$	$3.18 \cdot 10^{-4}$	$0.00 \cdot 10^{-3}$
Case II	$2.49 \cdot 10^{-4}$	$1.44 \cdot 10^{-2}$	$1.24 \cdot 10^{-3}$	$0.00 \cdot 10^{-3}$
Case III	-23.79	-10.29	-17.89	-13.68
Case IV	-23.79	-12.65	-10.99	-21.97

Table 4

Computational expense: total number of SQP iterations and computation time required to generate a Pareto front with 11 points for the different methods.

		SQP [-]			CPU time [s]		
		WS	NNC	NBI	WS	NNC	NBI
PWC	Case I	337	198	272	16.3	10.0	14.3
	Case II	351	235	266	40.6	29.4	34.4
	Case III	1203	429	231	74.0	23.3	17.4
	Case IV	1185	1500	458	73.4	92.9	32.5
AP	Case I	200	90	52	152.0	79.3	52.7
	Case II	293	170	92	362.8	210.6	141.2
	Case III	248	76	45	37.1	16.5	18.0
	Case IV	178	131	51	32.5	25.5	20.2

Variables

$\mathbf{b}_i$	vector of initial boundary conditions	
$\mathbf{b}_t$	vector of terminal boundary conditions	
$\mathbf{c}_p$	vector of path constraints	
$\mathbf{c}_t$	vector of terminal constraints	
C	reactant concentration	[mol/L]
C_F	reactant concentration in feed stream	[mol/L]
C_s	substrate concentration	[g/L]
$C_{s,F}$	substrate concentration in feed stream	[g/L]
c_p	specific heat of reactor fluid	[J/kg K]
D_C	mass dispersion coefficient	[m ² /s]
D_T	heat dispersion coefficient	[m ² /s]
d	reactor diameter	[m]
E	activation energy	[J/mol]
$\mathbf{f}$	vector of system equations	
g_i	terminal cost part of objective J_i	
ΔH	heat of reaction	[J/kmol]
h	heat transfer coefficient	[W/m ² K]
h_i	integral cost part of objective J_i	
$\mathbf{J} = [J_1, \dots, J_m]^T$	vector of objective functions	
$\bar{\mathbf{J}}$	vector of normalised objective functions	
$\mathbf{J}^*$	utopia point	
$\mathbf{J}_p$	point on the CHIM	
$\bar{\mathbf{J}}_p$	point on the normalised CHIM	
$\mathcal{J}$	feasible cost domain	
$\bar{\mathcal{J}}$	feasible domain of normalised objective functions	

J_i	i-th individual objective function	
$\bar{J}_i$	i-th normalised individual objective function	
$J_i^\diamond$	maximum value of the i-th objective for the set of all individual minimisers	
K	scaling factor	
k_0	kinetic constant	[1/s]
L	reactor length	[m]
R	ideal gas constant	[J/mol K]
T	reactor fluid temperature	[K]
T_F	temperature of feed stream	[K]
T_w	jacket fluid temperature	[K]
t	time	[h]
$\mathbf{u}$	vector of controls	
$\mathcal{U}$	feasible control domain	
$[\mathbf{u}_i^*, \xi_{f,i}^*]$	individual minimiser of the i-th objective J_i	
v	reactor fluid superficial velocity	[m/s]
$\mathbf{w}$	vector of weights	
w_i	i-th weight	
$\mathbf{x}$	vector of states	
z	spatial coordinate	[m]
ε	ε in the ε -constraint method	
λ	distance from point in the CHIM	
μ	specific growth rate	[1/h]
π	specific production rate	[g/g h]
ρ	reactor fluid density	[kg/m ³]
σ	specific substrate consumption rate	[g/g h]
Φ	pay-off matrix	
ξ	independent variable in ODEs	

Subscripts

min	value at its lower bound
max	value at its upper bound
i	index of a component in a vector
f	terminal value
$inside$	value inside the feasible region
$sing$	singular value
$path$	value determined by path constraint
tot	total weighted sum value

Superscripts

*	optimal value
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Acronyms

AP	analytical control parameterisation
CHIM	convex hull of individual minima
MOO	multiple objective optimisation
MOOC	multiple objective optimal control
NBI	normal boundary intersection method
NCO	necessary conditions of optimality
NNC	normalised normal constraint method
ODE	ordinary differential equations
PWC	piecewise constant control parameterisation
SQP	sequential quadratic programming
WS	weighted sum method