Chapter 4

Methodology II: processes with decaying performance

Non nova, sed nova

4.1 Introduction

In the previous chapter the set-points optimisation has been illustrated by using only external disturbances. Nevertheless, when a process is also affected by internal disturbances like fouling, catalyst deactivation and so on, the proposed approach is still being valid. On the one hand, RTE will react to the external disturbances as they enters to the plant. On the other hand, every time the steady state is reached, the effect of internal disturbances is also taken into account by means of model updating. The presence of process degradation posses, however, an additional issue: a mandatory periodical maintenance action, which is the subject of consideration of the current chapter.

Such problem is quite common in industrial practice. When the efficiency of equipment decreases with running time and/or with the amount of the different materials processed, appropriate measures should be taken to reestablish the initial performance level. The resulting decision-making problem consists in determining *when* such actions should be carried out, thus leading to a trade-off between the cost of the action itself (resources required, production break, etc.) and the expected benefit it generates (productivity increase, reduction of operational costs, etc.).

As detailed in chapter 2, many mathematical programming approaches have been proposed, both MILP (e.g. Georgiadis et al. (1999)) and MINLP (e. g., Alle et al. (2002); Tjoa et al. (1997) and Buzzi et al. (1984)), while little attention has been paid to the on-line management of the discrete decisions involved in processes with decaying performance. Specifically, it is usually ignored that the model updating module of an on-line optimisation system, or more generally, the

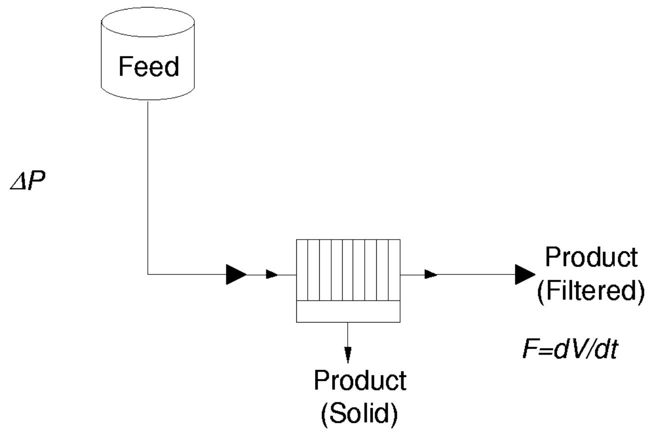

Figure 4.1: Simplified filter press scheme

distributed control system (DCS), may provide significant information about the process degree of performance and its variation with time.

In this chapter, a step forward to the integration of both approaches (conventional mathematical programming and on-line optimisation) is presented. A simple formulation (NLP) for the off-line planning problem is provided together with a procedure for the subsequent implementation of the discrete decisions involved (clean or not, feed assignments, etc.) in a real time environment. The proposed methodology is an extension of the Real Time Evolution (RTE) approach for continuous processes introduced in the previous chapter. Some examples are used to illustrate and validate the proposed approach for the planning procedure and the on line optimisation.

4.2 Motivating problem: example I

Consider a classical example of semi-continuous operation: filtration at constant pressure. Such situation is commonly found in practice when the feed is stored in a vessel located at some height above the filter (figure 4.1). During the filtration process, the filtration rate decreases continuously, because of the increase in the pressure drop associated to the solid accumulated on the filtration cake. At a given moment, the filtration must be interrupted in order to clean the filter, restoring then the initial situation. It is clear that there is a trade-off to when deciding such action. The bigger the cycle length, the lower the non-productive fraction of the whole cycle. However, a big cycle length decreases the average rate. Thus, it is worth knowing the instant that maximises the filtration capacity.

The classical off-line approach for dealing with such problem consists of obtaining the average capacity as a function of the time and then solving the associated maximisation problem, as is explained next.

Preliminary calculations:

The filtration is a unit operation that can be considered as a special case of fluid flow through a static granular (packed) bed. Because of the size of the particles is typically quite small, the flow regime is generally laminar. Consequently, the Ergun equation can be used, omitting the terms that correspond to the turbulent conditions:

$$f_p = \frac{150}{Re_p} \tag{4.1}$$

with:

$$\begin{aligned} Re_p &= \tfrac{d_p \upsilon_s \rho}{(1-\varepsilon)\mu} \\ f_p &= h_f \tfrac{\varepsilon^3}{(1-\varepsilon)} \tfrac{d_p}{L\upsilon_s^2} \end{aligned} \tag{4.2}$$

since for this case $h_f = \Delta P$, the following formula is obtained:

$$\frac{\Delta P}{L} = 150 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu}{\rho d_p^2} \upsilon_s \tag{4.3}$$

where:

Re_p: Reynolds' number for fluid flow through packed beds.

f_p: friction factor.

h_f: pressure drop associated to friction losses.

ΔP: pressure drop trough the filter.

L: length of the cake.

ε: cake void fraction.

μ: fluid viscosity.

d_p: equivalent diameter of the particles of the cake.

υ_s: fluid superficial velocity.

It should be noted that since the relationship of the equation 4.1 is dimensionless, the units of measure used in the equation 4.3 can be freely chosen while their consistency is kept.

Given that the values of the void fraction and the equivalent diameter of the particles constituting the cake change according to the material, and considering besides the definition of υ_s:

$$\upsilon_s = \frac{volumetric\ flow}{section} = \frac{1}{A_p}\frac{dV}{dt} \tag{4.4}$$

equation 4.3 can be rewritten in the simplified form:

$$\frac{1}{A_p}\frac{dV}{dt} = K_p\frac{\Delta P}{\mu L} \tag{4.5}$$

According to this equation, the superficial velocity (refereed to the area of the section normal to the flow, denoted by A_p) is directly proportional to the pressure difference between the upper and lower sides of the cake and inversely proportional to the fluid viscosity and cake length (depth). Since the length of the cake continuously increases during the filtration, and considering the constant resistance of the filtration media, equation 4.5 takes the form:

$$\frac{1}{A_p}\frac{dV}{dt} = K\frac{\Delta P}{\mu\left(\frac{\alpha\omega V}{A_p} + R_m\right)} \tag{4.6}$$

where:

A_p: is the section perpendicular to the flow.

V: total volume of filtrate.

α: specific cake resistance.

ω: feed concentration, expressed as the mass of solid per unit of volume filtered.

R_m: filtration medium resistance.

For the case of incompressible cakes, with constant pressure drop, equation 4.6 becomes (Ocon and Tojo, 1977):

$$\frac{dt}{dV} = a \cdot V + b \tag{4.7}$$

where:

$$a = \frac{\alpha\mu\omega}{A_p^2\Delta P} \tag{4.8}$$

$$b = a \cdot V_e = \frac{\alpha\mu\omega}{A_p^2\Delta P}V_e \tag{4.9}$$

In such case, the resistance offered by the filtration material is expressed as an hypothetical layer of cake corresponding to the volume V_e of the filtrated required to form such hypothetical layer:

$$R_m = \frac{\alpha\omega V_e}{A_p} \tag{4.10}$$

The computation of the constants a and b is made using experimental data, performed at constant pressure, of the filtered volume as function of time. The integration of the ordinary differential equation 4.7, using the condition $V = 0$ for $t = 0$ allows to obtain:

$$V = \sqrt{V_e^2 + \frac{2t}{a}} - V_e \tag{4.11}$$

Filtration capacity:

The filtration capacity (C_f) is defined by the ratio of the volume to filter to the total cycle time:

$$C_f = \frac{V(ts)}{ts + \tau_m} = \frac{\sqrt{V_e^2 + \frac{2ts}{a}} - V_e}{ts + \tau_m} \tag{4.12}$$

where ts and τ_m denote the productive and non-productive time of a cycle respectively. Thus, to maximise the capacity:

$$\left.\frac{dC_f}{dts}\right|_{ts=ts_{opt}} = \left.\frac{d\left[\frac{\sqrt{V_e^2+\frac{2ts}{a}}-V_e}{ts+\tau_m}\right]}{dts}\right|_{ts=ts_{opt}} = 0 \tag{4.13}$$

from where:

$$ts_{opt} = \tau_m + b\sqrt{\frac{2\tau_m}{a}} \tag{4.14}$$

or else:

$$V_{opt} = \sqrt{\frac{2\tau_m}{a}} \tag{4.15}$$

Figure 4.2 shows the graphical interpretation of such solution, a classical method for obtaining the optimal cycle length, not only for batch filtering but also many batch operations.

Numerical example:

As very simple numerical example, consider the case where a filtration is carried out at a constant pressure in a filter press. The cake is incompressible and the numerical values for the significant parameters are those of table 4.1. In order to obtain the optimal cycle length, equations 4.14 and 4.15 can be used, from where: $t_{opt} = 43\,min$ and $V_{opt} = 114\,L$.

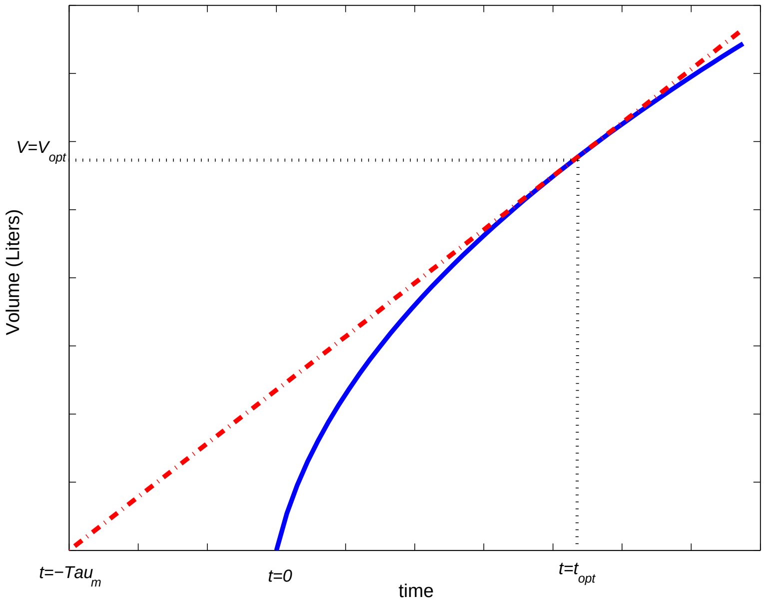

Figure 4.2: Classical graphical solution for ts_{opt} determination in the filtration example

Table 4.1: Data for a single filter

Parameter	*Value*
$a\ \left(10^3 min/L^2\right)$	4.58
$b\ \left(10^1 min \cdot L\right)$	1.13
$\tau_m\ (min)$	30

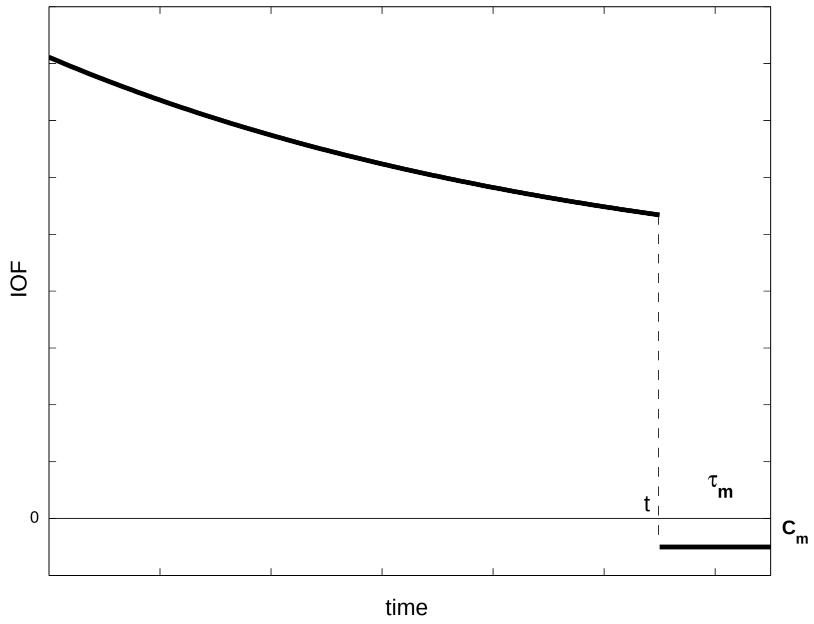

Figure 4.3: Typical evolution of IOF for a process with decaying performance

4.3 Off-line approach

4.3.1 Generalising the simplest case

Equations and analysis given in the previous section can be applied to many cases of common semi-continuous (cyclic) operations, not only filtration but also others like for instance ionic exchange, catalyst reactions with decreasing activity and evaporation, between others (i.e. Epstein (1979); Casado (1990); O'Donnell et al. (2001)). However, in a more general sense, the simplest case of maintenance problem corresponds to a single process whose performance (Instantaneous Objective Function, IOF) decreases with time. At some time ts, the operation must be finished in order to perform some maintenance task, which re-establishes the process initial conditions. The maintenance task consumes a known time τ_m and its corresponding cost is C_m (figure 4.3). It can be seen that the lower the time ts, the higher the performance but at the expense of the cost and time associated to the maintenance itself. Therefore, there is a trade-off in the determination of time ts, the question being the time, ts_{opt} that maximises the overall performance during the whole operating cycle.

Under such situation, the mean performance (Mean Objective Function, MOF) during the whole cycle will be given by the equation:

$$MOF(ts) = \frac{\int_0^{ts} IOF(\theta)d\theta - C_m}{(ts + \tau_m)} \tag{4.16}$$

which can be solved, in general terms, in an analytical way since the optimal maintenance time

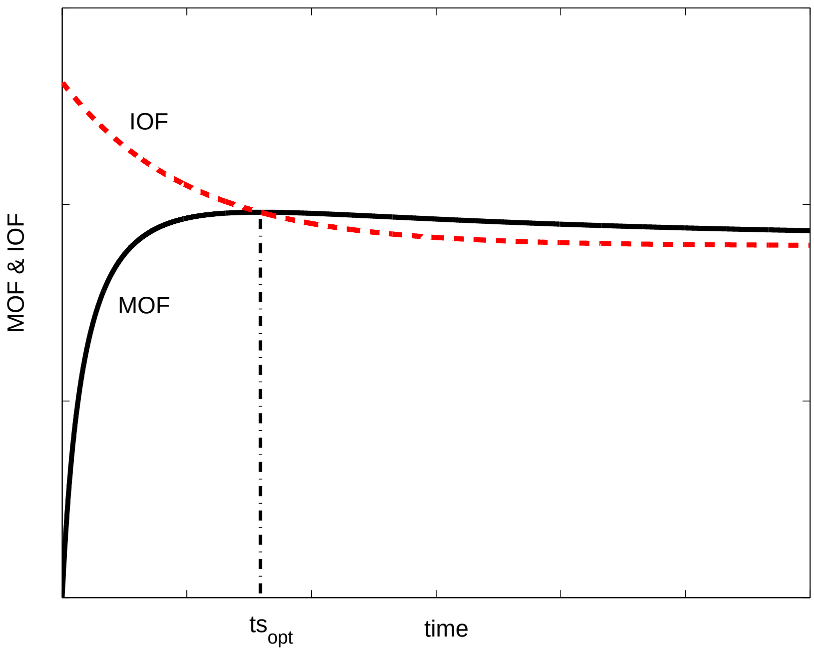

Figure 4.4: Graphical solution for any IOF decreasing with time

(ts_{opt}) must satisfy:

$$\left.\frac{dMOF(ts)}{dts}\right|_{ts=ts_{opt}} = \frac{IOF(ts_{opt})(ts_{opt}+\tau_m)+C_m-\int_0^{ts_{opt}} IOF(\theta)d\theta}{(ts_{opt}+\tau_m)} = 0 \tag{4.17}$$

to obtain:

$$IOF(ts_{opt}) = \frac{\int_0^{ts_{opt}} IOF(\theta)d\theta - C_m}{(ts_{opt}+\tau_m)} = MOF(ts_{opt}) \tag{4.18}$$

Therefore, using an appropriate model for IOF the optimum policy can be found (figure 4.4). It should be noted, that ts_{opt} corresponds to that time which makes the value of $IOF(ts)$ equal to the value of $MOF(ts)$ (Buzzi et al., 1984).[1]

For the filtration case considered in the example I:

$$IOF = \frac{dV}{dts} = \frac{1}{k(V+V_e)} \tag{4.19}$$

and

[1]In many practical situations, the maintenance action takes place when a condition related to the process safety is meet. An example of this case would be a reaction shut down triggered when the pressure reaches a threshold level.

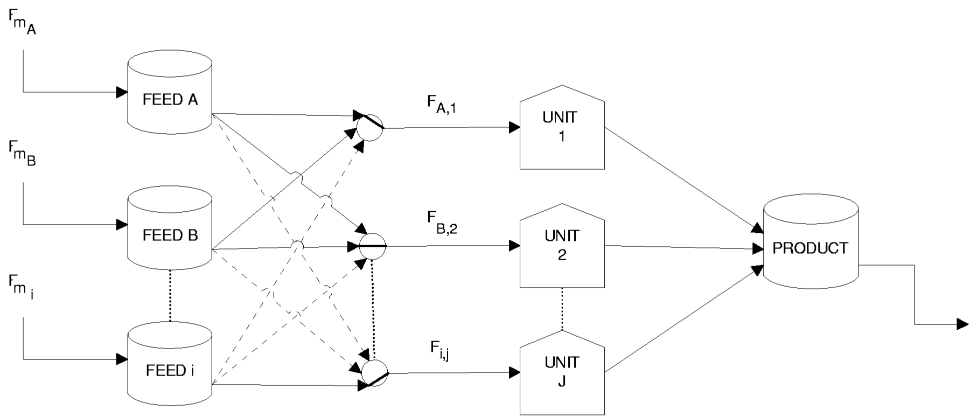

Figure 4.5: Scheme for the general case considered

$$MOF = \frac{V}{ts + \tau_m} \tag{4.20}$$

From where the equations 4.14 and 4.15 can be easily obtained by using the equation 4.17. Note that such procedure allows to manage not only the maximum capacity case, but also any other with economical basis which may also include the cleaning task cost.

4.3.2 The effect of different feeds and units

As has been previously explained, the operation of units with decaying performance must be interrupted in order to perform a maintenance operation. Therefore, and aiming a smooth production output, plant equipment is often run in parallel. Furthermore, it may be also possible to count with several available feeds. Figure 4.5 illustrates a possible situation. Such conditions motivate the existence of additional constraints related to the mass balance, besides possible bounds in the processing rates.

In such context, the general problem to be considered can be stated as follows. There are $i = 1 \ldots I$ feedstock available to produce the final product P (see figure 4.5). The total average consumption of every feed F_{m_i}, should be between a lower and an upper bound, $F_{m_{lo_i}}$ and $F_{m_{up_i}}$. There are $j = 1 \ldots J$ parallel units available to process these feeds, whose performance for processing every feed (Instantaneous Objective Function, $IOF_{i,j}$) decreases with the operating time (ts). Let the maintenance operations costs and duration be $C_{m_{i,j}}$ and $\tau_{m_{i,j}}$ respectively.

Additionally, suppose that whenever there is a feed changeover, maintenance tasks take place, and the operating parameters are set in such a way that the unit returns to operate at the best possible conditions for the next feed. Therefore, the objective of this problem is to find the duration of the cycles ($ts_{i,j}$) for every pair feed-unit and the corresponding feed flows to be processed (F_{m_i}).

Assume that the unit j operates consuming feed i at a rate $F_{i,j}$ during a time $ts_{i,j}$ (sub-cycle time for feed i, unit j). During that time, the Instantaneous Objective Function will be a function of $ts_{i,j}$:

$$IOF_{i,j} = f(ts_{i,j}) \tag{4.21}$$

Then, the corresponding Mean Objective Function (MOF) during the whole sub-cycle for every pair feed-unit will be given by:

$$MOF(ts) = \frac{Total\ Benefits - Maintenance\ Costs}{Total\ Cycle\ Time} = \frac{\int_0^{ts} IOF(\theta)d\theta - C_m}{(ts + \tau_m)} \tag{4.22}$$

Let $Tf_{i,j}$ be the time fraction of unit j operation dedicated to the processing of feed i. Then, the average consumption of feed i (F_{m_i}) can be expressed as a function of $Tf_{i,j}$ at each unit j:

$$F_{m_{i,j}} = \sum_j F_{i,j} \frac{ts_{i,j}}{ts_{i,j} + \tau_{m_{i,j}}} Tf_{i,j} \tag{4.23}$$

Then, a NLP formulation for this family of problems is proposed as follows:

$$\max_{ts_{i,j},\, Tf_{i,j}} \quad Z = \sum_i \sum_j MOF_{i,j} \cdot Tf_{i,j} \tag{4.24}$$

subject to:

$$MOF_{i,j} = \frac{\int_0^{ts_{i,j}} IOF_{i.j}(\theta)d\theta - C_{m_{i,j}}}{\left(ts_{i,j} + \tau_{m_{i,j}}\right)} \quad \forall i,j \tag{4.25}$$

$$F_{m_i} = \sum_j F_{i,j} \frac{ts_{i,j}}{ts_{i,j} + \tau_{m_{i,j}}} Tf_{i,j} \quad \forall i \tag{4.26}$$

$$\sum_i Tf_{i,j} = 1 \quad \forall j \tag{4.27}$$

$$F_{m_{lo_i}} \leq F_{m_i} \leq F_{m_{up_i}} \quad \forall i \tag{4.28}$$

$$0 \leq Tf_{i,j} \leq 1 \quad \forall i,j \tag{4.29}$$

$$ts_{lo} \leq ts_{i,j} \leq ts_{up} \quad \forall i,j \tag{4.30}$$

where:

$MOF_{i,j}$: Mean Objective Function (monetary units/time).

$IOF_{i,j}$: Instantaneous Objective Function (monetary units/time).

$C_{m_{i,j}}$: maintenance cost (monetary units).

$\tau_{m_{i,j}}$: time devoted to maintenance (time).

$Tf_{i,j}$: time fraction of unit j devoted to process feed i (time/time).

$ts_{i,j}$: operating time for the pair feed-furnace (time), bounded by ts_{lo} and ts_{up}.

$F_{i,j}$: feed rate of feed i to unit j during the operating time ts (flow basis).

Sub-indexes i and j refer to the feed and the unit respectively. The problem has $2 \cdot i \cdot j$ degrees of freedom, being the corresponding decision variables the operating times ($ts_{i,j}$) and the time fractions ($Tf_{i,j}$), the later related directly to the average feed flows ($F_{m_{i,j}}$).

4.3.3 Validation benchmarks

These examples are based in the work reported by Jain and Grossmann (1998). The case studies contemplate different feeds that are available for arriving continuously to storage tanks at a constant rate, like those illustrated in figure 4.5. All feedstock are then processed sequentially in a set of reactors (the furnaces), where as a consequence of coking, the conversion decreases with time according to the equation:

$$Y_{i,j} = c_{i,j} + a_{i,j} e^{-b_{i,j} ts_{i,j}} \tag{4.31}$$

where a, b and c are empirical parameters.

Additionally, it is assumed that the income is directly proportional to production, and the proportionality constant is given by the price parameter $P_{i,j}$. This parameter takes into account the revenues obtained by selling the product and all the expenses incurred for producing it, except the cleanup cost. Therefore, the problem consists in determining the operating policy that maximises the profit.

The following sub-section considers a relatively simple case, with only one furnace, while the next one considers also the possibility of feed-unit allocation. In both cases, the formulation proposed by the mentioned authors is included as a reference, for comparison purposes.

4.3.3.1 One unit-several feeds: example II

Three different feeds (A, B, C) that are available for arriving continuously to the corresponding storage tanks at a constant rate (figure 4.6). Specific data for the example considered are found in table 4.2.

Jain and Grossmann (1998) have proposed a problem formulation (*F1*), based on the following variables:

t_i: total processing time of feed i to the furnace.

n_i: number of sub-cycles of feed i in furnace during the total cycle time.

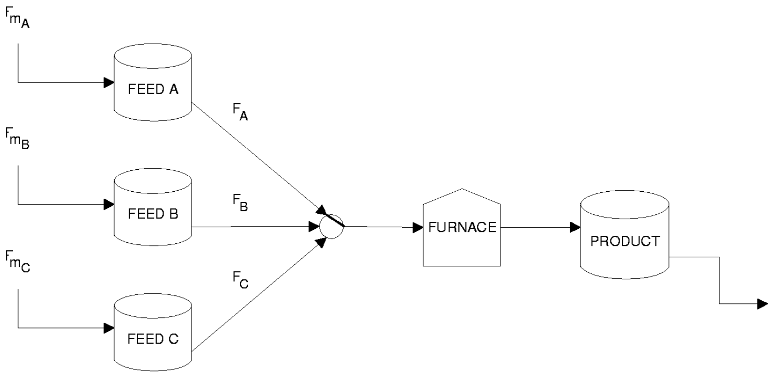

Figure 4.6: Example II scheme

Table 4.2: Data for example II

Parameter	Feed *A*	Feed *B*	Feed *C*
$\tau_{m_i}(d)$	2	3	3
$F_i(t/d)$	1300	1000	1100
a_i	0.20	0.18	0.19
$b_i(1/d)$	0.10	0.13	0.09
c_i	0.18	0.10	0.12
$P_i(\$/t)$	160	90	120
$C_{m_i}(\$)$	100	90	80
$F_{m_{lo_i}}(t/d)$	350	300	300
$F_{m_{up_i}}(t/d)$	650	300	300

Table 4.3: Example II solution (*F1*)

Variable	Feed *A*	Feed *B*	Feed *C*
n_i	4	1	2
$t_i(d)$	42.44	41.74	37.94
$ts_i(d)$	10.61	41.74	18.97
Tf_i (%)	36.26	32.16	31.59
$F_{m_i}(t/d)$	396.6	300.0	300.0
$T_{cycle}(d)$	139.1		
$Z(\$/d)$	30430		

F_{m_i}: feeding rate of the feed i (denoted by F_i in the original paper).

Δt_i: total feeding and cleanup time associated to feed i.

T_{cycle}: total cycle duration (denoted by T_c in the original paper).

Z: average profit during the total cycle.

where, the decision variables are: t_i, n_i and T_{cycle}. Since all constraints can be linearised, the resulting MINLP problem can be solved using an NLP-based Branch and Bound (taking care to avoid division by zero in the terms with $\frac{t}{n}$ of the objective function). As shown by Jain and Grossmann (1998), the global optimum will be found since the constraints are linear and the objective function is pseudo-convex (pseudo-concave). The solution reported is shown in table 4.3.

This formulation has some disadvantages. Firstly, the solution is strongly dependent on arbitrary upper bounds used for T_{cycle} and n_i. The reported solution corresponds to the upper bounds of 4 for n_i and 140 *days* for T_{cycle}. But, for higher values of T_{cycle} and n_i upper bounds, the dependence still continues. For instance, when the bounds for n_i and T_{cycle} are 6 and 200 respectively, the optimal objective function value increases to 30507, and so on.

Hence, a different formulation (*F2*) is used instead, in accordance with the general case:

$$max\,Z = \sum_i MOF_i \cdot Tf_i \tag{4.32}$$

subject to:

$$MOF_i = \frac{P_iF_i\left[c_its_i + \frac{a_i}{b_i}\left(1 - e^{-b_its_i}\right)\right] - C_{m_i}}{(ts_i + \tau_{m_i})} \quad \forall i \tag{4.33}$$

$$F_{m_i} = F_i\frac{ts_i}{ts_i + \tau_{m_i}}Tf_i \quad \forall i \tag{4.34}$$

$$\sum_i Tf_i = 1 \tag{4.35}$$

Table 4.4: Example II solution† (*F2*)

Variable	Feed A	Feed B	Feed C
$ts_i(d)$	9.76	60.00	21.34
Tf_i (%)	37.39	31.50	31.11
$F_{m_i}(t/d)$	403.5	300.0	300.0
$MOF_i(\$/d)$	53109	10547	23656
$Z(\$/d)$	30549		

†Starting from random initial points the same solution is reached

$$F_{m_{lo_i}} \leq F_{m_i} \leq F_{m_{up_i}} \quad \forall i \tag{4.36}$$

$$0 \leq Tf_i \leq 1 \quad \forall i \tag{4.37}$$

$$ts_{lo} \leq ts_i \leq ts_{up} \quad \forall i \tag{4.38}$$

In this formulation, the decision variables are the ts_i and Tf_i (or alternatively F_{m_i}). Now, the optimal solution is summarised in table 4.4.

From the results given in table 4.3 and table 4.4, the following conclusions can be drawn:

- The second formulation (*F2*) gives a better Z value for the same problem. The main reason is that there is no bound related to the finite cyclic operation (T_{cycle} variable and associated constraints).
- In both cases, the contribution to profit (MOF's) obtained processing raw materials A and C is substantially higher than processing B.
- The lower bound constraints on feeds B and C are active.

The interpretation of these results is quite straightforward. In the absence of lower bounds for F_{m_B} and F_{m_C} the obvious solution would be to process only the feed A (i.e. the most profitable one) with its ts satisfying the equation 4.18 (the best one) whenever the F_{m_A} upper bound allows it. As this is not the case, ts_B (i.e. the less profitable feed) is set to ts_{up}, thus "forcing" the required feed consumption as soon as possible. Besides, the value of ts_C is such that allows processing the minimum required feed and makes the time fraction summation equal to one.

4.3.3.2 Several units-several feeds: example III

The scenario for this case study corresponds to the general case of the previous example and has been also excerpted from the previously mentioned work. Now, four furnaces and seven feeds are considered. The corresponding parameters are given in table 4.5, while table 4.6 shows the corresponding solution using *F1*, (T_{cycle} about 35 d and Z of $1.654 \cdot 10^5\,\$/d$).

Table 4.5: Data for example III

Parameter	Furnace j	Feed i						
		A	B	C	D	E	F	G
$\tau_{m_{i,j}}(d)$	1	2	3	3	3	1	2	3
	2	3	1	2	2	2	1	1
	3	1	3	1	1	2	1	2
	4	2	1	3	2	2	1	1
$F_{i,j}(t/d)$	1	1300	1200	1100	800	1300	300	700
	2	1100	1050	1000	1000	1200	400	600
	3	900	800	800	1200	1000	300	850
	4	1200	1000	800	700	1200	400	600
$a_{i,j}$	1	0.30	0.40	0.35	0.32	0.29	0.35	0.31
	2	0.32	0.38	0.33	0.31	0.28	0.40	0.34
	3	0.31	0.35	0.36	0.36	0.29	0.37	0.31
	4	0.31	0.36	0.35	0.36	0.28	0.39	0.32
$b_{i,j}(1/d)$	1	0.10	0.20	0.10	0.20	0.23	0.34	0.20
	2	0.20	0.10	0.20	0.25	0.29	0.27	0.30
	3	0.30	0.20	0.30	0.27	0.28	0.29	0.25
	4	0.20	0.20	0.15	0.25	0.29	0.22	0.28
$c_{i,j}$	1	0.20	0.18	0.21	0.20	0.30	0.26	0.16
	2	0.21	0.19	0.23	0.25	0.31	0.27	0.17
	3	0.19	0.18	0.21	0.23	0.30	0.25	0.18
	4	0.20	0.19	0.21	0.24	0.31	0.26	0.17
$P_{i,j}(\$/t)$	1	123	105	110	123	105	110	120
	2	114	132	129	114	132	129	113
	3	110	122	120	110	122	120	117
	4	120	125	129	115	115	128	115
$C_{m_{i,j}}(\$)$	1	100	90	80	75	90	93	78
	2	80	85	75	90	94	78	70
	3	90	90	90	85	93	92	75
	4	80	90	85	80	92	85	72
$F_{m_{lo_i}}(t/d)$		300	400	300	500	500	100	600
$F_{m_{up_i}}(t/d)$		600	700	600	800	800	400	900

Table 4.6: Example III solution (*F1*)

Feed (i)	$F_{m_i}(t/d)$	Profit (%)‡	Furnace (j)	$n_{i,j}$	$t_{i,j}(d)$
A	353	10.32	1	1	9.55
B	700	26.62	2	4	23.55
C	300	8.69	1	1	9.57
D	500	14.28	3	3	14.70
E	800	24.97	1	2	9.07
			2	1	5.65
			4	1	8.13
F	100	3.34	4	1	8.84
G	600	11.77	3	1	15.62
			4	2	13.18
$T_{cycle}(d)$	35.42				
$Z(\$/d)$	165400				

‡Profit is expressed as percentage of Z

Table 4.7: Example III solution (*F2*)

Feed (i)	$F_{m_i}(t/d)$	Profit (%)⋆	Furnace (j)	$ts_{i,j}(d)$	$Tf_{i,j}$ (%)
A	389	19.3	1	8.71	36.78
B	700	13.4	2	5.25	79.38
C	300	8.8	1	12.87	15.06
			2	8.15	20.63
D	500	14.9	3	4.48	50.96
E	800	28.9	1	4.79	48.16
			4	7.96	29.40
F	100	3.1	4	7.51	28.33
G	600	11.6	3	20.00	49.04
			4	6.79	42.27
$Z(\$/d)$	166500				

⋆Profit is expressed as percentage of Z

On the other hand, the proposed formulation, *F2*, has been used to obtain the results of table 4.4. It is worth noting that given the non-linearity of the problem, it has been solved from 200 random (uniformly distributed) initial points. It takes about 0.2 seconds to solve every problem.[2]The histogram of figure 4.7 shows the relative frequency of the local optima objective function values, which are expressed as percentage of the best one. It can be seen that most of the optima found fall in a favourable region. In fact, using the binomial probability distribution function, one may verify that the probability of reaching the best solution is 99.99% starting only from 10 independent initial points. Table 4.7 summarises the results of the best solution (using ts_{up} equal to 20 *days*).

By comparing the solution reached (table 4.7) with that obtained using *F1* (table 4.6), the following considerations can be drawn:

[2]In a AMD-K7 processor with 128 Mb RAM at 600 MHz, using CONOPT2 solver in the GAMS environment (Brooke et al., 1998; Drud, 1992). About 2 seconds in an spreadsheet environment using an implementation of GRG2 (Fylstra et al., 1998).

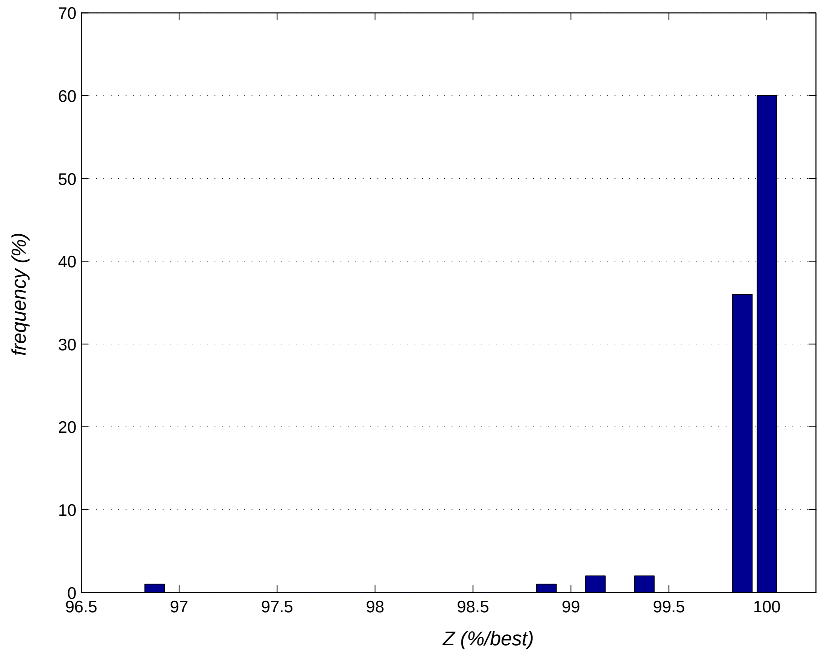

Figure 4.7: Histogram of the different solutions obtained using *F2* for the Example III

- The objective function value obtained using the proposed formulation *F2* is higher. That can be explained because in the proposed formulation the cyclic operation corresponds to every furnace rather than to the whole system.
- The computation time is substantially reduced because there are no integer variables to compute in the proposed formulation.

Additionally, it should be mentioned that the lower bounds for feeds C, D, F and G, and the upper bounds for B and E, and ts_{up} for G-3 are the active constraints. Besides, note that ts_{A1} corresponds to that obtained using equation 4.18.

4.4 On-line approach

During the process design stage, $IOF(t)$ is usually expressed as a function of operating conditions, and it is embedded in the remaining equations that describe the process. For example, catalyst activity is commonly expressed as an additional kinetic expression. This expression can be included with others describing the reactor operation, and therefore the solution of the whole system of differential equations allows the computation of the corresponding $IOF(t)$.

For the sake of simplicity, the previous examples models have assumed simple empirical relationships which allowed a direct $IOF(t)$ calculation (e. g. parameters a, b and c) rather than by solving a complex set of differential equations. However, for some complex situations found in practice the use of such empirical models may fail. Regarding this issue, Schulz et al. (2000)

have shown the effects using more refined models (including recycle streams) on the planning decisions made at an existing ethylene plant.

Thus, in a general sense, there are two main reasons for disagreement between modelling results and the actual values obtained in plant:

The plant-model mismatch: that may lead to "bad" values of the model parameters (i.e. a, b and c). This behaviour might be caused, for instance, by unexpected disturbances, inadequate model updating procedure and frequency, and so on. Furthermore, it could be actually originated by some strong structural model error.

Variability in the model parameters: since model parameter values are commonly determined by statistical techniques, and they are just averaged values. Therefore, the instantaneous plant behaviour will be different from run to run (cycle to cycle). Such variability magnitude is approximately given by the degree of deviation observed during the parameter adjustment stage.

Hence, the results of applying mathematical programming approaches will vary according to the implementation methodology, because the previous factors will have more or less influence on the global behaviour. Therefore, an alternative approach is desirable for finding ts_{opt} and Tf_{opt} on-line.

Fortunately, there is another way to evaluate $IOF(t)$. A common expression for IOF is in terms of profit, measured as the value of products less the raw material and operation costs. When adequate sensors are available (Sánchez and Bagajewicz, 2000), the components of this expression can be computed. For instance, the production quantity and quality, raw materials and utility consumption are usually available from the Distributed Control System (DCS), and Plant Information Systems, and therefore the IOF can be calculated on-line by incorporating the corresponding economic parameters (prices, cost factors, etc.). In this context, an alternative approach for on-line optimal maintenance management is proposed, based also on plant data rather than only on the decaying performance model. Basically, the on-line optimisation problem consists of a set of very simple questions formulated periodically, and is addressed to the identification of eventual incremental improvements.

In fact, it is essentially the same idea introduced in the previous chapter for the on-line optimisation of continuous processes. However, the variant introduced takes fully advantage of the monotonically changing behaviour by implicitly embedding the process model into the on-line decision-making technique. The proposed on-line strategy is next introduced using the examples given in section 4.3 (page 77).

4.4.1 Simplest case: example I

Assume that:

- The information needed to compute IOF at every time interval k is available on-line.

- The function $IOF(k)$ is strictly decreasing with time.

Under such circumstances, it is known (figure 4.4 in page 78) that there exists a unique optimal time interval k_{opt} for performing the corresponding maintenance task. According to that, instead of solving the corresponding optimisation problem, one can solve a simpler one by answering the following question at every period k: Should one stop for maintenance at this period or at the next one?

The answer can be obtained just by comparing $MOF(k)$ and $MOF(k+1)$, at every interval k. Naturally, if $MOF(k) < MOF(k+1)$ it is better to wait. Otherwise, when $MOF(k) \geq MOF(k+1)$ then it is better to stop at period k (see figure 4.4). It can be observed that this is equivalent to compute:

$$MOF(k+1) - MOF(k) = 0 \tag{4.39}$$

which is the discrete form of the equation 4.17, and hence provides the optimal solution.

This statement may hold, even when C_m and τ_m are available as a function of the operating time instead of constant values. An interesting extension of the proposed strategy for continuously obtaining a good estimation of the maintenance time from on-line data is detailed in the appendix C (page 193).

In order to illustrate the application of this technique, consider example I, where the off-line optimal solution for the available data (table 4.1) corresponds to $ts_{opt} = 30\,min$. Regarding the first hypothesis, note that for this example the IOF can be readily obtained from on-line flow measurements. On the other hand, the second hypothesis is somehow intrinsic to the problem (because if IOF does not decrease with time, the problem does not exist).

Then, in order to apply the proposed strategy, it is assumed, for the sake of simplicity that both plant-model mismatch and variability from cycle to cycle can be emulated using the following equation:

$$p_\pi = p_{\pi_{nom}} \cdot [1 + \sigma \cdot INVNS(rand) + \xi] \tag{4.40}$$

where:

$p_{\pi_{nom}}$: nominal parameter value.

p_π: parameter value used in the model (changing for every sub-cycle).

σ: standard deviation for nominal parameter value (to emulate variability).

ξ: relative error in the nominal parameter value (to emulate plant-model mismatch).

$rand$: uniformly distributed random number.

$INVNS$: inverse of the normal standard cumulative distribution.

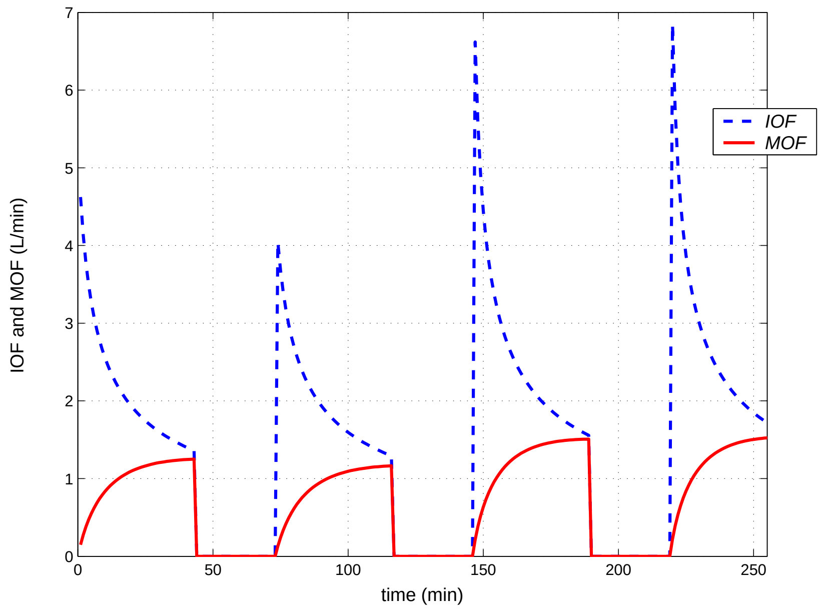

Figure 4.8: Strict implementation of off-line results

For this problem, p_π refers to the empirical parameters a and b. In such conditions, the strict implementation of the off-line result over a dynamic simulation (where the values of σ and ξ are pre-specified) will lead to the results shown in figure 4.8.[3] It can be seen, that fixing ts, a frequency distribution of MOF values is obtained, where cleaning tasks are carried out when $IOF \neq MOF$.

However, under the same conditions of plant-model mismatch and variability, when ts_{opt} is determined on line according to the proposed RTE strategy much better performance is achieved, as is shown in figure 4.9. Note that the on-line determination of the optimality condition (i.e $IOF(ts_{opt}) = MOF(ts_{opt})$, according to equation 4.18) may not necessarily lead to the same ts_{opt} value obtained off-line.

Figure 4.10 shows the resulting distribution of the on-line ts_{opt} obtained for $\xi = -10\,\%$ and $\sigma = 10\,\%$, where the off-line value is included as a reference. Again, like in the previous case, a frequency distribution for MOF is obtained.

With the aim of obtain an approximate measure of the potential benefits of implementing the proposed on-line approach, a Monte Carlo simulation for different values of ξ and σ is performed (equation 4.40). The difference between the performances (expected value for MOF) of both approaches is used as comparative index, leading to the results shown in figure 4.11. As expected, the on-line determination of ts_{opt} always enhances the process performance and the higher the plant-model mismatch (or variability), the higher the improvement. For this particular example, the approximate improvement is about 2500 liters/year in terms of filter capacity (for $\sigma \approx 20\,\%$ and $\xi \approx 10\,\%$). Considering that usually such kind of equipment is run in parallel, among several

[3] ts_{opt} is fixed in this case, but V_{opt} could be fixed instead.

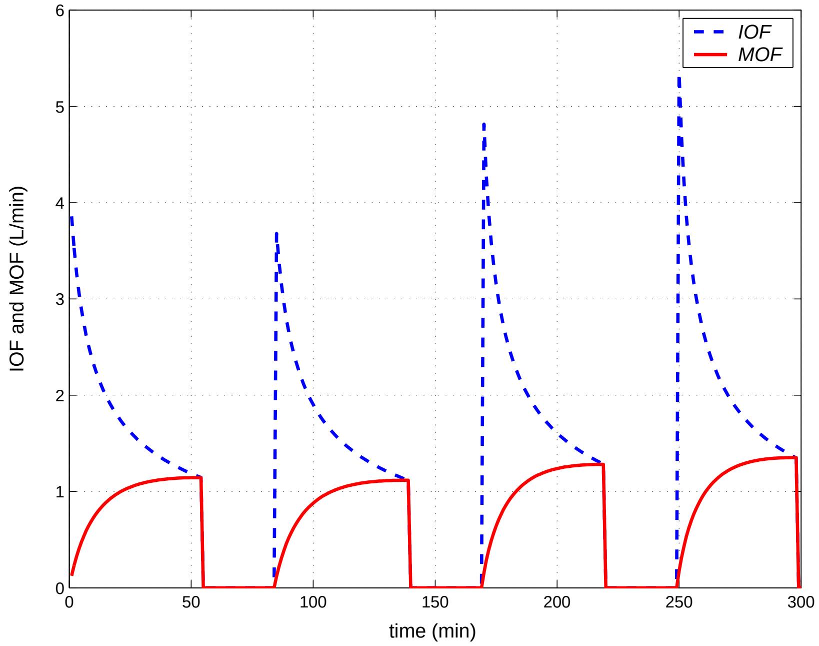

Figure 4.9: On-line determination of cycle lengths

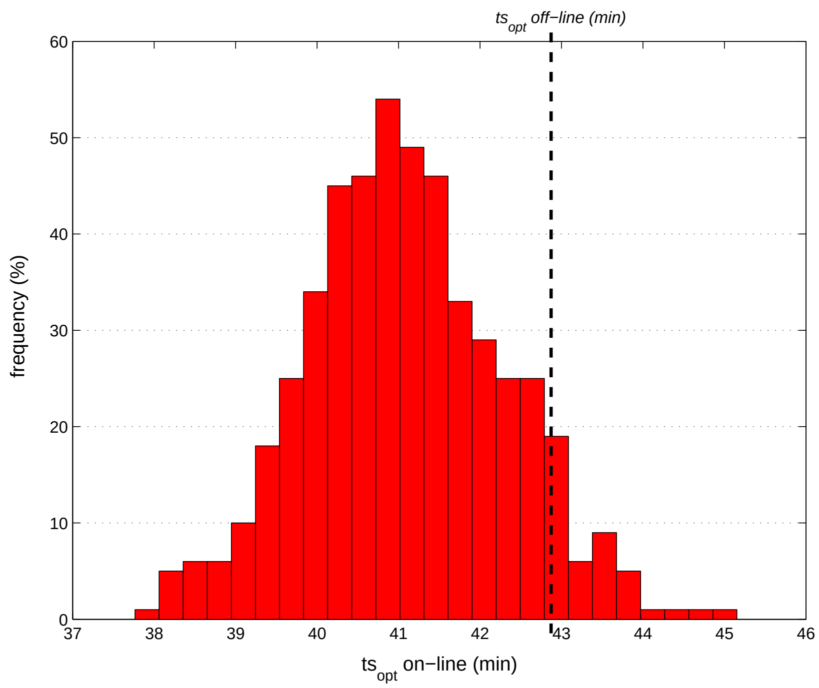

Figure 4.10: Example I. Histogram for ts_{opt} for $\xi = -10\,\%$ and $\sigma = 10\,\%$

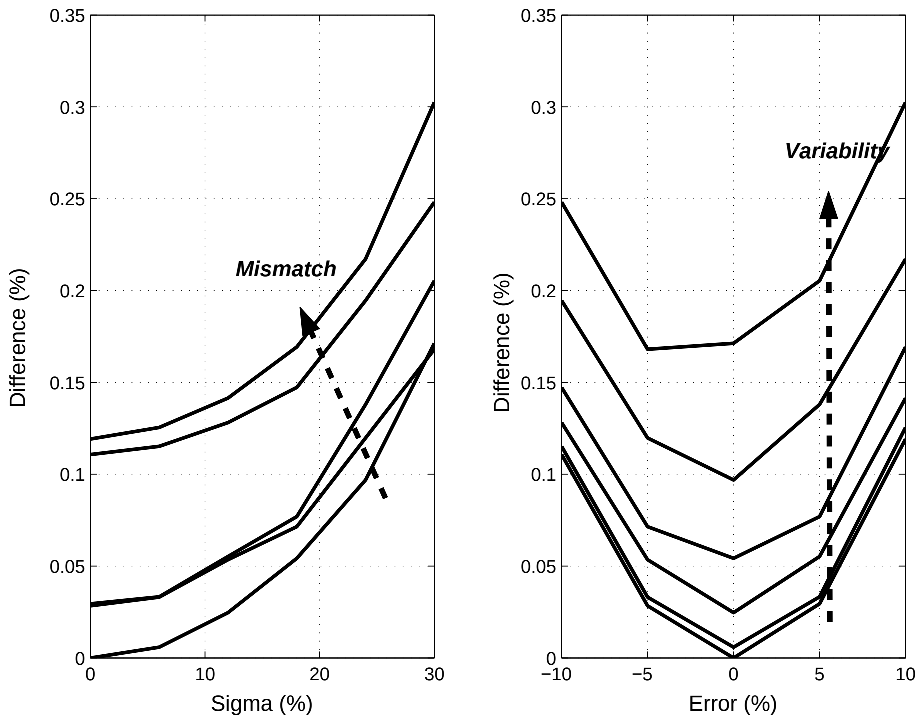

Figure 4.11: Example I. Improvement reached applying RTE over different plant-model mismatch and variability conditions

ones, the on-line determination of cleaning tasks may be economically compensated.

4.4.2 One unit-several feeds: example II

For the second example, the off-line solution offers significant information that also gives an opportunity for on-line optimisation. Specifically, the flow assignments resulting from the off-line optimisation (model) correspond to a "first stage" decision. Once implemented such decision, the optimal operating times (ts_i) can be determined as the information from the plant becomes available. Originally in this example, there were six degrees of freedom (three Tf's and three ts's). Assuming that the three F_m's are identified using the off-line solution, there only remain three decision variables. In addition, ts_B is the maximum allowed and the equation 4.35 forces the material balance to be satisfied, so that only one degree of freedom remains. This degree of freedom corresponds to ts_A variable, which can be determined on-line using the procedure explained in the previous section.

However, it is important to mention that the ts_A variability obtained by its on-line determination will change the corresponding Tf_A. Therefore, in order to insure that the implemented solution satisfies the mass balance, ts_C needs to be also recalculated from cycle to cycle, according to (from equation 4.35):

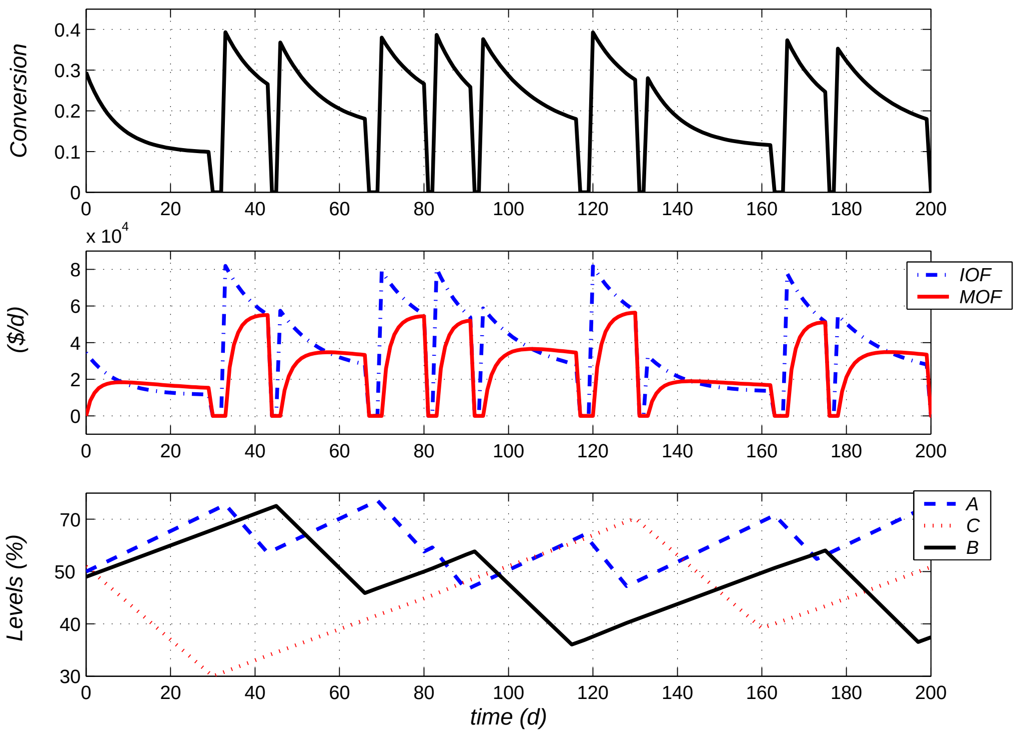

Figure 4.12: Example II. Use of RTE for on-line optimisation ($ts_{up} = 30\,d$)

$$T f_C = 1 - T f_A - T f_B$$
$$ts_C = \frac{\tau_{m_C} F_{m_{lo_C}}}{\left(F_C T f_C - F_{m_{lo_C}}\right)} \tag{4.41}$$

where $T f_A$ is obtained from $T f_A = \frac{ts_A + \tau_{m_A}}{ts_A} \frac{F_{m_A}}{F_A}$ (from equation 4.34), and ts_A is updated (and damped) from cycle to cycle.

In order to select the feed to be next provided to the furnace after the cleaning is finished, a simple selection rule can be used (just choosing the material having the highest inventory level) and thus the $T f_i$ decision variables are automatically implemented. Figure 4.12 shows the application of the explained strategy over a dynamic model.

Additionally, the benefits of the proposed approach when plant-model mismatch and variability are present have been approximated as in example I by means of a long-term Monte Carlo simulation. In this case, the parameters a, b, and c were changed using the equation 4.40. The results are given in the graphics of figure 4.13.

The influence of the variability σ is more significant than that for the error ξ, as it could be expected, because the variability is the main motivation for on-line optimisation systems. Charts of the type of figure 4.13 are very useful for the economic evaluation of a RTE system project, given that by properly approximating the variability and the plant-model mismatch one is able to estimate the benefits of such on-line optimisation system.

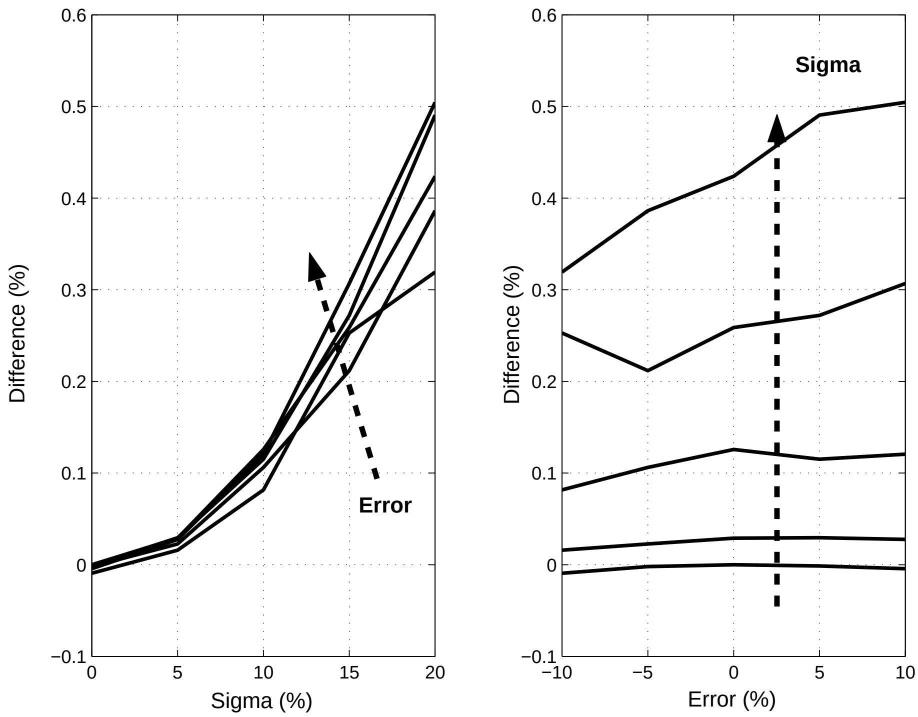

Figure 4.13: Example II. Improvement reached applying RTE

4.4.3 Several units-several feeds: example III

The application of similar concepts also permits the on-line approach to this problem, and the larger number of variables and constraints allows generalising the previous concepts. The original formulation has $Tf_{i,j}$'s and $ts_{i,j}$'s as decision variables, which means 56 degrees of freedom. However, the consideration of the flow assignments and results from the off-line optimisation, implies 48 additional equations:

$$F_{m_i} = \sum_j F_{i,j} \frac{ts_{i,j}}{ts_{i,j} + \tau_{m_{i,j}}} Tf_{i,j} \quad \forall i \tag{4.42}$$

$$Tf_{i,j} = 0 \Rightarrow ts_{i,j} = 0 \, \forall (i,j) \in \left\{ \begin{array}{l} (A,2);(A,3);(A,4); \\ (B,1);(B,3); \\ (C,3);(C,4); \\ (D,1);(D;2);(D,4); \\ (E,2);(E,3); \\ (F,1);(F,2);(F,3) \\ (G,1);(G,2) \end{array} \right\} \tag{4.43}$$

$$\sum_i Tf_{i,j} = 1 \quad \forall j \tag{4.44}$$

$$ts_{i,j} = ts_{up}\ (i,j) = \{(G,3)\} \tag{4.45}$$

which means that the remaining degrees of freedom are 8. After some algebraic manipulation (Lee et al., 1966) all the dependent variables ($Tf_{i,j}$'s and ts_{G4}) can be expressed as a function (mostly using the mass balances) of an independent set of $ts_{i,j}$'s variables: ts_{A1},ts_{B2},ts_{C1},ts_{C2} ,ts_{D3},ts_{E1}, ts_{E4} and ts_{F4}. In addition, in that resulting reduced space, the optimum point must satisfy:

$$\frac{\partial Z}{\partial ts_{m,n}} = 0\ \forall (m,n) \in \left\{ \begin{array}{l} (A,1); \\ (B,2); \\ (C,1);(C,2); \\ (D,3); \\ (E,1);(E,4); \\ (F,4) \end{array} \right\} \tag{4.46}$$

what can be rewritten in the form:

$$\begin{gathered} \frac{\partial\left[MOF_{m,n}(ts_{m,n})Tf_{m,n}(ts_{m,n})\right]}{\partial ts_{m,n}} = \\ = -\left\{ \sum_{\substack{i\neq m \\ j\neq n}} MOF_{i,j}\frac{\partial Tf_{i,j}(ts_{m,n})}{\partial ts_{m,n}} + \sum_{\substack{i\neq m \\ j\neq n}} \frac{\partial MOF_{i,j}(ts_{m,n})}{\partial ts_{m,n}} Tf_{i,j} \right\} \\ \forall (m,n) \in \left\{ \begin{array}{l} (A,1); \\ (B,2); \\ (C,1);(C,2); \\ (D,3); \\ (E,1);(E,4); \\ (F,4) \end{array} \right\} \end{gathered} \tag{4.47}$$

where:

$$ts_{i,j} = ts_{opt_{i,j}}\ \ \forall (i,j) \neq (m,n) \tag{4.48}$$

This set of equations completes the system for the on-line solution.

Therefore, when feeding the furnace n with the feed m, the on-line measurement of $IOF_{m,n}$ allows obtaining $MOF_{m,n}$ continuously. Besides $Tf_{m,n}$ is determined from $ts_{m,n}$ using the mass balances. That allows computing the LHS (equation 4.47) as a function of $ts_{m,n}$'s on-line.

On the other hand, the RHS is a function of $ts_{m,n}$ that can be easily evaluated numerically. All $MOF_{i,j}$'s are obtained from the historical optimal values (using as initial value the off-line result) and the $Tf_{i,j}$'s values (for $i,j \neq m,n$) are computed from the mass balances equations using also the historical $ts_{opt_{i,j}}$'s values.

Figure 4.14 shows the evolution of the Z_i values along time (different $ts_{m,n}$) where the plant

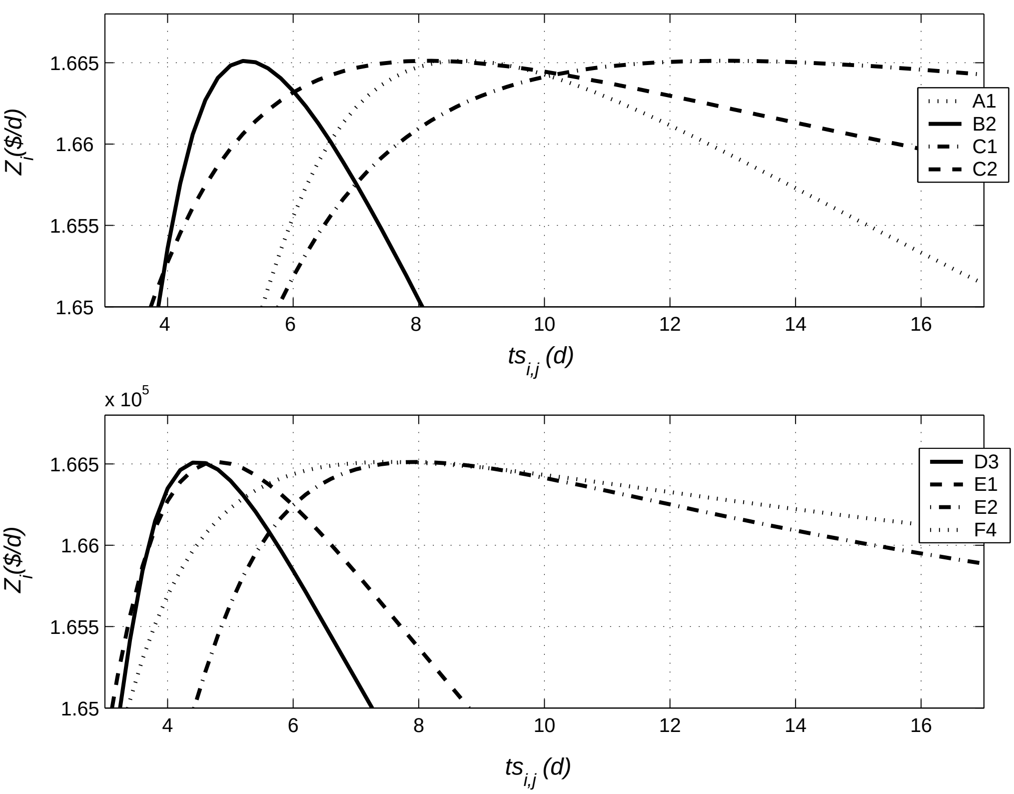

Figure 4.14: Example III. On-line determination of ts_{opt}

was not stopped in order to clearly illustrate the Z_i profiles and how the optimum values may be identified on-line. It should be noted, that special care must be taken given that commonly, for lower $ts_{i,j}$ values, values for some dependent variables ($Tf_{i,j}$ and the remaining $ts_{i,j}$ $\forall(i,j) \neq (m,n)$) become negative and hence correspond to infeasible solutions.

Regarding the on-line implementation of $Tf_{i,j}$ variables, the reasoning presented in the previous example holds. However, the contribution of every feed to every furnace needs to be considered. One way to easily do this is by splitting the real inventory into "pseudo-inventories" for every furnace. The split fractions ($Sf_{i,j}$) for this computation are based on the additional terms in equations 4.26:

$$F_{m_{i,j}} = \sum_j F_{i,j} \frac{ts_{i,j}}{ts_{i,j} + \tau_{m_{i,j}}} Tf_{i,j} = \sum_j Sf_{i,j} F_{m_i} \quad \forall i \tag{4.49}$$

Using for its evaluation the actual values obtained for $ts_{opt_{i,j}}$ and performing a normalisation periodically to ensure that:

$$\sum_j Sf_{i,j} = 1 \quad \forall i \tag{4.50}$$

The procedure presented is quite general, and its application to the previous example (example II) produces similar results to those obtained in the previous section. However, it is important to notice that, in the case of example III, the improvement reached using an on-line optimisation is not much relevant. This is not surprising, since the solution reached is mainly given by the satisfaction of mass balance constraints (lower an upper bounds in F_{m_i}'s) which does not leave enough margin for the on-line manipulation of the $ts_{m,n}$'s variables.

4.5 Conclusions

The work introduced in this chapter represents a step forward towards the integration of classical mathematical formulations for the maintenance planning of processes with decaying performance and the on-line optimisation technology. A way for the off-line calculation of a maintenance plan and a methodology for the on-line implementation of such planed decisions in a co-ordinated way have been presented. The main advantages of the proposed approach are its simplicity and robustness, which makes it attractive for industrial application in process plants provided with information systems.

Moreover, the proposed NLP formulation includes general performance relationships and mass balances, which allows its use over a wide range of applications. The variables involved have a clear physical meaning, and the computation times required are indeed affordable. What is more important is the fact that the solutions are easy to implement, and even more, they can be further used for performing on-line optimisation. Otherwise, the proposed procedure for on-line optimisation is quite simple, robust and reduces the effects of plant model mismatch and variability. The RTE strategy has proved to obtain good solutions by using properly the information coming from the plant and answering simple questions on line, rather than performing successive formal optimisation, which has been the commonly used strategy. The on-line procedure seems to be especially worthwhile in cases with highly decreasing performance rates and where the off-line optimal solution is not strongly dictated by the constraints.

4.6 A short comment about the simultaneous implementation of both RTE methodologies

The previous chapter has introduced a methodology conceived as a strategy for reaching and keeping a hypothetical moving optimal operation point. This is achieved by a proper periodical modification of the set-points, which constitute a set of continuous variables. It has been designed with the aim of dealing particularly with the continuous arrival of external disturbances. Nevertheless, as previously argued, the fact that the models are updated during the steady state operation allows as well pursuing, with a lower rate, possible internal changes. Fortunately, the rate of change for internal disturbances is in general terms lower, in order of magnitude, as compared with the external disturbances changes.

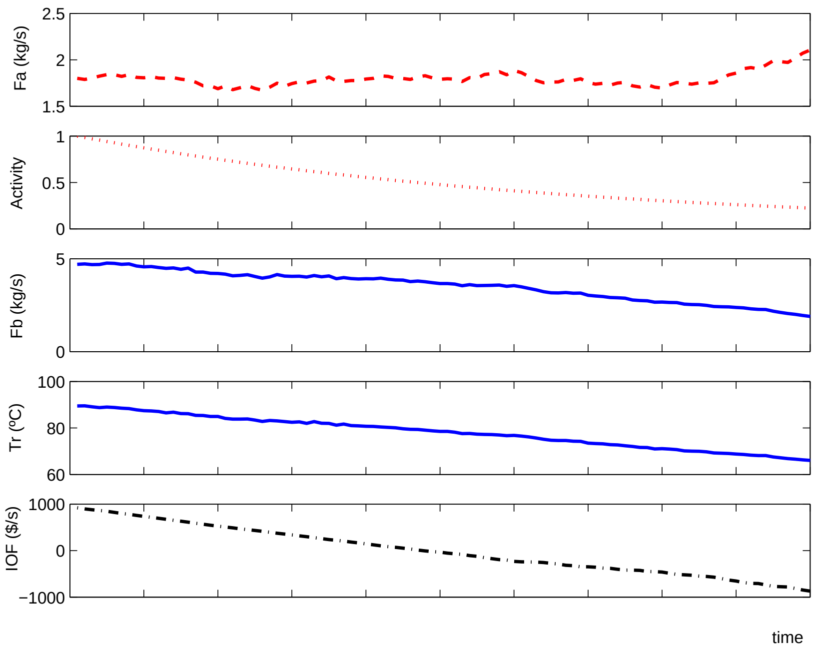

Figure 4.15: Set-points optimisation for the Williams-Ottto reactor under the simultaneous influence of internal and external disturbances

In addition, this chapter has introduced another methodology conceived for the on-line optimisation of process with decaying performance. It takes advantage of the a priori knowledge of the disturbance trend and the fact that at some instant the operation must be interrupted in order to restore the initial performance. The question that naturally arises is if both methodologies are suitable for being applied simultaneously over the same process.

Consider for illustration purposes the Williams-Otto reactor benchmark, when now, the main reaction is a catalytic one. Furthermore, assume that as a consequence of poisoning, the catalyst's activity continuously decreases. Such situation clearly corresponds to an internal disturbance. In addition, during its operation, and as has been considered in previous analysis, another disturbance (external) is present: the feed flow of the A reactant. If under such context, the methodology introduced in chapter 3 is applied, the set-points of F_b and T_r will track the drifting optimum, as is shown in figure 4.15. In the figure, only the points corresponding to the steady state (actually pseudo steady states) are displayed.

It can be seen in the chart at the bottom, the corresponding evolution of IOF, which results decreasing with time. There is no reason for not implementing, in a parallel way, the methodology of the current chapter. Indeed, if the cost associated to the catalyst regeneration and the required non-productive time are properly specified (C_m and τ_m), and besides, there are mechanisms for evaluating IOF on-line, the procedure of section 4.4 (page 87) can be readily applied. Indeed, 4.16 shows the optimal operation time when arbitrary values of C_m and τ_m are supposed.

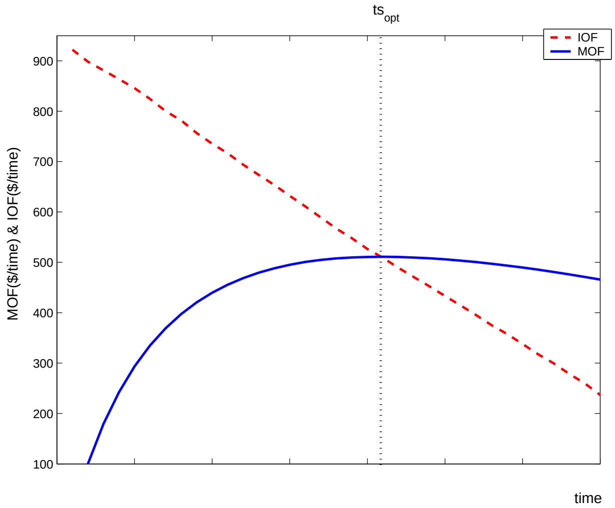

Figure 4.16: Determination of ts_{opt} for the Williams-Ottto reactor under the simultaneous influence of internal and external disturbances