This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Zakharov, A.; Jämsä-Jounela, Sirkka-Liisa

Iterative optimization of the economic efficiency of an industrial process within the validity area of the static plant model and its application to a Pulp Mill

Published in:
Computers and Chemical Engineering

DOI:
[10.1016/j.compchemeng.2010.10.010](https://doi.org/10.1016/j.compchemeng.2010.10.010)

Published: 01/01/2011

Document Version
Peer reviewed version

Please cite the original version:
Zakharov, A., & Jämsä-Jounela, S-L. (2011). Iterative optimization of the economic efficiency of an industrial process within the validity area of the static plant model and its application to a Pulp Mill. *Computers and Chemical Engineering*, 35(2), 245-254. <https://doi.org/10.1016/j.compchemeng.2010.10.010>

This material is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

Iterative optimization of the economic efficiency of an industrial process within the validity area of the static plant model and its application to a Pulp Mill

A. Zakharov*, S.-L. Jämsä-Jounela
Aalto University, P.O. Box 16100, 00076, Aalto, Finland

Abstract

Optimization of the steady state economic efficiency of an industrial process is a specific task because the decision variables of the optimization (setpoints of the control system) affect the process through the control strategy. Thus, the effects of saturation of a control system must be taken into account when the gradient of the objective function is estimated and the necessary optimality conditions are checked. In particular, because the optimality conditions cannot be checked directly in the presence of active constraints on the manipulated variables, approximations of the steady state values of the manipulated variables as functions of the setpoints (static plant model) are needed in order to be able to evaluate the optimality conditions. In this paper an iterative method for optimization of the plant profit rate is proposed avoiding the control saturation and is applied to the Pulp Mill benchmark model optimization. Three different static models describing the steady state values of the manipulated variables are constructed and used in the optimization. The results of the optimization are presented and compared against the straightforward single-step optimization of the plant economic efficiency.

© 2010 Elsevier Ltd. All rights reserved

Keywords

Plantwide optimization, Economic efficiency, Pulp and paper production, Industrial application

1 Introduction

Due to the continuously increasing competition in the pulp and paper industry, there is a need to develop solutions that can increase the economical efficiency of the plants. According to [Luyben \(1989\)](#) it is usually much cheaper, safer and faster to conduct the optimization of plant operations on the basis of a mathematical model rather than experimentally. However, the significant number of studies is still concentrated on the optimization of single unit operations in Pulp Mills: [Mcdonough, Uno, Rudie, and Courchene \(2008\)](#) studied the optimization of the ClO₂ requirements for the bleaching process; [Tang, Wang, He, and Itoh \(2007\)](#) optimized the Pulp Washing process; [Sarimveis, Angelou, Retsina, Rutherford, and Bafas \(2003\)](#) optimized the energy management in pulp and paper mills; [Smith, Christlmeier, and Van Winkle \(1986\)](#) studied the possibility of increasing of the recovery boiler throughput; [Sidrak \(1995\)](#) optimized the Kamyr Digester towards significant reduction in the amount of off-specification pulp. [Klugman, Karlsson, and Moshfegh \(2007\)](#) studied the energy consumption and production by the Pulp Mill; [Savulescu and Alva-Argaez \(2008\)](#) minimize the energy consumption through managing the direct heat transfer related to the water streams; [Westerlund et al. \(1986\)](#) solved the equilibrium equations for the white liquor and optimized the lime feed rate; [Santos and Dourado \(1999\)](#) optimized energy consumption and the plant's production; [Thibault et al. \(2003\)](#) concentrated their efforts on the multicriteria optimization of the plant.

Nowadays, the trend is to optimize the whole mill with respect to production and quality, minimization of energy, chemical consumption and effluents. In a recent paper [Castro and Doyle \(2004\)](#) have proposed the Pulp Mill benchmark model, having the standard architecture with a Kamyr digester, a bleaching plant and a chemical recovery (see [Castro and Doyle \(2004\)](#) for the details). The benchmark model is well suited for

[Type here]

performing of a wide range of the Pulp Mill studies, including the optimization problem of economical efficiency. Recently Mercangöz and Doyle (2008) have performed the optimization of the benchmark model, which deals with the whole Pulp Mill and the optimization criterion is the plant's profit rate including energy costs, cooking and bleaching chemicals costs, final products sales (pulp and steam) and which takes into account delignification and brightness requirements to the final product. However the optimization is performed in a single iteration and the simulation results are relatively far from the prediction of the static model. The attempt to update the model bias and re-optimize the plant (the bias update procedure) is not able to improve the profit rate, even though the updated model promises a significant increase in profits.

The inability of the bias update procedure to improve the profit rate may be explained by the fact that the static process model constructed in the area free of control saturation is invalid in the presence of active constraints on the manipulated variables. In addition, convergence of the iterative optimization implemented on the basis of the bias update procedure cannot be ensured and, in practice, convergence may not be reached. An iterative optimization method is proposed in this paper, which is free of the described drawbacks and provides convergence of optimization to the point where the approximated optimality conditions, introduced in the paper, are fulfilled.

The article is structured as follows: Section 2 contains a description of the iterative optimization method together with the approximated optimality conditions. Section 3 introduces the Pulp Mill benchmark model and formulation of the profit rate maximization problem. Section 4 contains the results of computations for both one-step and iterative optimizations. Finally, Section 5 contains the discussion and conclusions.

2 Iterative optimization of the economic efficiency of an industrial process under the validity limitations of the static plant model

2.1 Problem formulation

In the chemical industry, the control is organized in a hierarchical structure: at the lowest level measurements (such as temperatures, pressures and flows) are collected and the basic control loops are implemented in order to stabilize the plant. The next level includes advanced regulatory controllers such as MPC and cascade controls. At the subsequent level, short-term decisions are made by the real time optimization, which mainly adapts the process to the changing measurable and immeasurable disturbances. At the highest level, long-term optimization is performed which takes into account plant-wide planning and scheduling, as well as the plant static model. At this level the process conditions are controlled through the setpoint U (see Fig. 1), which plays a role of the decision variables of the optimization. Profit rate computation in the chemical industry mainly utilizes the steady values of the manipulated variables V_j which are functions of the setpoints:

$$V_j = F_j(U), \quad j = 1, \dots, m.$$

Both the setpoints and the manipulated variables are limited by the following constraints, which are caused by the physical limitations of the plant and the stability requirements of the control system:

$$\begin{aligned} l_i^u &\leq U_i \leq h_i^u, \quad i = 1, \dots, n \\ l_j^u &\leq V_j \leq h_j^v, \quad j = 1, \dots, m. \end{aligned} \tag{1}$$

In fact, functions F_j may demonstrate non-smooth behavior arising from saturation of the control. Let the plant setpoint be varied smoothly. At the moment when a manipulated variable (MV) used by a control loop reaches its limit, the control strategy no longer follows its setpoint, thereby immediately affecting to

[Type here]

the rest of the process. If a MV used by a MPC becomes saturated, then the controller continues to try to keep the process at the setpoint by means of the other variables at its disposal. Thus, in both cases many MV's (not only the MV used by the control loop) demonstrate non-smooth behaviour at the moment of control loop saturation. Obviously, functions F_j are smooth inside the set S of the setpoints, within which the manipulated variable constraints are inactive:

$$S = \{U: l_j^v < F_j(U) < h_j^v, \quad j = 1, \dots, m\}.$$

Fig. 1. Schematic diagram of the process

2.2 Approximated optimality conditions

An efficient optimization is hardly possible without easy-to-check optimality conditions. The necessary optimality conditions are based on the gradient of the objective function, which is difficult to estimate at the border of the region S . Thus, approximate optimality conditions based on the static model of the process must be used.

Let us consider the following representation of the steady values of the manipulated variables in set S :

$$V_j = F_j(U) = f_j(U) + e_j(U), \quad (2)$$

where the set of functions, f_j , is the static model constructed and valid within S , and e_j are the approximation errors. In particular, the errors e_j can be estimated at a setpoint where the correspondent MV values are known and assumed to be constant.

The optimality conditions at the setpoint U for the profit rate maximization problem are standard Karush–Kuhn–Tucker conditions involving both derivatives $(\partial V_j / \partial U_i)|_U$ and values $V_j(U)$ of the manipulated variables. At the same time, optimization of the economic efficiency involves computation of the gradient of the profit rate with respect to the decision variables, which requires estimation of the derivatives $\partial V_j / \partial U_i$. Since these derivatives cannot usually be computed explicitly, they must be estimated using the following finite difference approximation:

$$\left. \frac{\partial V_j}{\partial U_i} \right|_U = \frac{V_j(U + \Delta_i) - V_j(U - \Delta_i)}{2\Delta}, \quad (3)$$

where Δ_i is the vector with the only non-zero element at the i th place, which is equal to Δ . If both points $U - \Delta_j$ and $U + \Delta_j$ belong to S , then the error of estimation (3) is of the order Δ^2 . However if $U + k\Delta_i$ is at the border of S for some k such that $-1 < k < 1$, then the manipulated variables are not smooth functions of the setpoints (as explained before), and the finite difference estimation is close to the linear combination of the left and right derivative at the point lying on the border of S :

$$\frac{V_j(U + \Delta_i) - V_j(U - \Delta_i)}{2\Delta} = \frac{1-k}{2} \left. \frac{\partial V_j}{\partial U_i} \right|_{(U+k\Delta_i)^+} + \frac{1+k}{2} \left. \frac{\partial V_j}{\partial U_i} \right|_{(U+k\Delta_i)^-} + O(\Delta).$$

[Type here]

To conclude, the finite difference estimation cannot be used as a reliable approximation of the derivative $(\partial V_j)/(\partial U_i)|_U$ if some of the MV constraints are active or close to be active. Since the simulations are able to provide only approximate steady state values of the MVs, a relatively large variation step Δ should be used to achieve a satisfactory level of accuracy. This is the reason why the gradient can be accurately estimated only ‘deeply’ within region S .

The gradient based optimization methods face a considerable challenge because of the above-mentioned problems with the derivative estimation. In fact, it is natural to expect that the iterative optimization will come to the border of the optimization region after only a few iterations, at which time a satisfactory solution has probably not yet been found. Thus, a method is needed that is suitable for the specific problem of plant optimization.

Since the values of the manipulated variables can be taken from the real process, or accurately estimated at any setpoint by means of a single simulation of a first principles process model, the only barrier for the optimality condition check are the derivatives $(\partial V_j)/(\partial U_i)|_U$ that cannot be estimated. One option is to use the approximated optimality conditions utilizing the approximation derivatives $(\partial f_j)/(\partial U_i)|_U$, which can be obtained analytically, instead of the $(\partial V_j)/(\partial U_i)|_U$. In particular setpoint U^* satisfies the approximated optimality condition, if the optimization of the profit rate with respect to model (2) with the constant error estimated at U^* returns U^* as the optimal solution. The approximated optimality conditions are almost equivalent to the original ones if the following estimation is fulfilled with a small positive ε :

$$\left| \frac{\partial e_i}{\partial U_j} \right|_U < \varepsilon.$$

Next, three different methods for constructing the approximations are briefly discussed.

2.3 Approximation methods of the manipulated variables

2.3.1 The linear approximation

Often the most pairs of the manipulated variables and decision variables produce dependences that can be described satisfactory with the simple linear approximation model as follows:

$$V_i \approx V_i^0 + \sum_j K_{i,j}(U_j - U_j^0), \quad (4)$$

where V_i , U_j are the i th manipulated variable and j th decision variable, and V_i^0 , U_j^0 , are their nominal values. The elements of the matrix $K_{i,j}$ are defined as partial derivatives of the manipulated variables with respect to the decision variable:

$$K_{i,j} = \left. \frac{\partial V_i}{\partial U_j} \right|_{U^0}.$$

The elements of $K_{i,j}$ are identified using a number of the plant tests and setpoints changes. Let consider the following setpoints:

- the nominal steady state with the j th component that has been stepped up by $+\Delta$,
- the nominal steady state with the j th component that has been stepped down by $-\Delta$.

[Type here]

The values of the manipulated variables at these steady states are denoted as V_i^u and V_i^l . At the next step, the finite difference estimation is used:

$$K_{i,j} = \frac{V_i^u - V_i^l}{2\Delta}. \quad (5)$$

In fact, two simulations for every decision variable are needed (a step above and a step below from the nominal value of the corresponding decision variable), totally ending up $2n$ simulations.

2.3.2. The one dimensional quadratic approximation

As an alternative to the linear technique, one can use the following approximation of a manipulated variable, promising the increase of the accuracy:

$$V_i \approx V_i^0 + \sum_j K_{i,j}(U_j - U_j^0) + 0.5 \sum_j L_{i,j}(U_j - U_j^0)^2. \quad (6)$$

All elements of matrix K (the matrix of the first derivatives) can be computed as it has already been described in the linear approximation approach section. In order to compute elements of matrix L (which are the second order derivatives of the manipulated variables with respect to the decision variables) it is necessary to perform two simulations with the following setpoints:

- the nominal steady state with the j th component that has been stepped by $+\Delta$,
- the nominal steady state with the j th component that has been stepped by $-\Delta$.

The values of the manipulated variables at these steady states are denoted as V_i^u and V_i^l . At the next step, the finite difference estimation for the second order derivatives is used:

$$L_{i,j} = \frac{V_i^u + V_i^l - 2V_i^0}{\Delta^2} \Big|_{U^0}. \quad (7)$$

The larger variations of the decision variables are needed compared to the linear model identification because the denominator in Eq. (7) is Δ^2 instead of 2Δ in Eq. (5). Since the same steady state values can be used in order to compute the elements of both matrixes K and L , it is still necessary to perform two simulations per each decision variable.

2.3.3. The multidimensional quadratic approximation

Finally, the third way can be used: every manipulated variable can be approximated by a multidimensional quadratic function of all decision variables:

$$V_i \approx V_i^0 + \sum_j K_{i,j}(U_j - U_j^0) + 0.5 \sum_{j,k} M_{i,j,k}(U_j - U_j^0)(U_k - U_k^0). \quad (8)$$

Actually, the approach includes all terms from the previous one, since the one dimensional quadratic terms are covered by the case j equals k . This way promises the most accurate approximation, however it requires a lot of computations to perform. For further let denote this approach as the multidimensional quadratic approach.

[Type here]

In this approach it is necessary to estimate the 3-dimensional matrix M . In order to do it, one has to perform one simulation for simultaneous variations of each pairs of the decision variables. Since there are $n(n + 1)/2$ pairs, it is necessary to perform $n(n + 1)/2$ of simulations.

2.4. Iterative optimization method

After the models of the MVs have been constructed, the solution of the optimization can be found in a single step if the errors of the model e_j are neglected. However, the obtained setpoint does not meet the approximated optimality conditions presented in Section 2.2 since, at the optimal point, the static model provides only approximate values of the manipulated variables. Thus an iterative method is obviously needed to find the setpoint satisfying the approximated optimality conditions.

It was explained in Section 2.1 that the approximation constructed within the constraint free region S is not valid in the presence of active constraints. As the result, the iterative optimization method must keep all the MV constraints inactive (otherwise the invalid gradients will be used and the optimization may stick at a point, which is far from the optimal one, without the possibility to improve it). The current solution of the optimization must be allowed to approach the constraints gradually, resulting in the optimal solution being found as the limit of the sequence of the inner points of region S . To ensure the convergence of the method a step coefficient is added to the iterative optimization.

Finally, the following iterative optimization method is proposed:

1. The MVs are described by linear or quadratic models f_j . The coefficients C_{con} and C_{step} are initialized with positive numbers. The current solution $U(0)$ is placed in the mid-point x^0 of the feasible region, where the approximation of the MVs is constructed. The vector of the model errors $E(0)$ is set at 0. The setpoint violation threshold st is then determined and the iteration number k is set to 0.
2. The simulation is performed at the current setpoint $U(k)$ and its results are used to estimate the steady values of the MVs $\bar{V}(k)$ and the controlled variables $\bar{U}(k)$.
3. The modeling error is estimated at the current solution point $U(k)$:

$$E_j(k) = \bar{V}_j(k) - f_j(U(k)), \quad j = 1, \dots, n,$$

and the model is updated:

$$V_j(U) \approx f_j(U) + E_j(k), \quad j = 1, \dots, n,$$

4. Conditions (1) are updated in order to keep the setpoint within region S :

$$l_j^v + C_{con} \leq V_j \leq h_j^v - C_{con}, \quad j = 1, \dots, m,$$

5. The optimal solution U^* of the problem of the profit rate maximization with respect to model (8) under the updated conditions is found. The next iteration setpoint is found as $U(k + 1) = (1 - C_{step})U(k) + C_{step}U^*$.
6. Step number k is increased by 1. Steps 2–6 are repeated while coefficient C_{con} slowly decreases towards to 0.

[Type here]

3 The Pulp Mill benchmark problem

3.1 Process description

In the Pulp Mill benchmark model developed by [Castro and Doyle \(2004\)](#) the chemical process units are modeled as perfectly mixed vessels or distributed parameters systems (plug flow vessels). Mass and energy balances are combined with the empirical equations for physical properties or thermodynamic information. The model has been implemented in C language in the form of SIMULINK program.

The process is composed of the two major sections: the fiber line and the chemical recovery loop. The objective of the fiber line is to convert woodchips into the pulp by a chemical process, which removes the lignin component from the woodchips. The main delignification is achieved in the unit, which is called the Kamyr digester. The remaining part of the fiber line is known as a bleaching plant. There the aim is to continue the delignification process, but also to remove the brown color. The color is represented by the brightness value, which is controlled by the optimization. In the benchmark problem, the bleaching process consists of three sequential towers D1, E0 and D2, where letters D and E symbolize the bleaching chemicals ClO_2 and NaOH , respectively. The quality criteria are specified for the Kappa number after the E-tower and the brightness after the D2-tower.

The second section in the Pulp Mill benchmark is the recovery loop, where the chemicals used in the fiber line are regenerated through a sequence of unit operations. The fresh reactive mixture used in the fiber line is known as white liquor. The mixture, leaving the digester is denoted as weak black liquor, which consists of reacted inorganic salts and the extracted organic components from the woodchips. The weak black liquor is concentrated in a series of evaporators and burned in the recovery boiler to utilize the heat content. The regeneration of NaOH is achieved in a series of causticizing reactions by using CaO . In a separate regeneration loop, CaO is recovered from the causticizing product CaCO_3 in a rotary Lime Kiln. As a result the recovery line makes the Pulp Mill process economically feasible.

3.2 Description of the control strategy

The optimization of the economical efficiency is highly related to the control of the plant. The plant-wide control is provided with the benchmark Pulp Mill model, which includes both the MPC and the SISO control loops. In the control strategy four MPC blocks control the most important variables in the Kamyr Digester (MPC1), Bleaching plant (MPC2), Chemical recovery (MPC3) and the Lime Kiln (MPC4). The general scheme is presented in [Fig. 2](#).

MPC controllers regulate 14 important quality and environmental variables. A number of SISO controllers are used to stabilize the open-loop unstable modes of the process and the rest are used to maintain the process conditions in various unit operations. The setpoints of the basic control loops are partly generated by the MPC and partly defined as inputs of the plant. In addition, 21 manipulated variables are not used for any process control purposes.

Since the setpoints that are given to the MPC, most of the setpoints of the basic controllers and some manipulated variables of the model can be freely varied and used as decision variables for the economical optimization of the Pulp Mill. According to [Mercangöz and Doyle \(2008\)](#), the following 44 variables (denoted as U) presented in [Table 1](#) are used for the optimization in the study.

Since the optimization of the economical efficiency is based on the steady state of the plant only, the dynamics of the plant during its path to a steady state are not studied.

[Type here]

The next step is to find the corresponding steady state of the Pulp Mill and to compute its economical efficiency. The steady state (further nominal steady state that will be used as an initial approximation for the economical efficiency optimization) can be easily found via performing a simulation with a long time horizon with the setpoints, defined by values of the decision variables. The nominal values of the following economically significant variables are thus defined and presented in Table 2.

Fig. 2. Scheme of the Pulp Mill control strategy

Most of the economically significant variables (denoted as V) are the manipulated variables of the Pulp Mill (the only exceptions are the pulp production rate and steam production rate), expressed in a volumetric or mass flow rate. Both decision and economically significant variables are scaled, thus most of scaled variables have lower and upper limits equal -1 and $+1$. The costs of all the chemicals are presented in Table 3.

Table 1

List of the decision variables

Short name	Variable name	Related to	Lower bound	Nominal value	Upper bound
U1	D2 production rate	MPC1	629.979	629.998	630
U2	Digester kappa	MPC1	12.5	19.9993	26
U3	Digester upper EA	MPC1	2.399	9.59977	16.799
U4	Digester lower EA	MPC1	2.25	9.00007	15.75
U5	Upper extract conductivity	MPC1	17.46	69.8423	122.224
U6	Lower extract conductivity	MPC1	12.11	48.4702	84.822
U7	O kappa	MPC1	7	9.99972	15
U8	E kappa	MPC2	2.4	2.5	2.6
U9	E washer [OH]	MPC2	0.0004499	0.00085	0.0012499
U10	D2 brightness	MPC2	0.8	0.81	0.84
U11	Black liquor solids	MPC3	0.625	0.65001	0.675
U12	Slaker temperature	MPC3	669.012	674.012	679.012
U13	Kiln O ₂ excess %	MPC4	0.0149	0.03497	0.0549
U14	Kiln CaCO ₃ residual %	MPC4	0.02487	0.02487	0.02487
U15	Digester liquor temperature	SISO	425.5	435.5	445.5
U16	O tower temperature	SISO	368	371	373.55
U17	D1 tower temperature	SISO	329	339	347.4999
U18	E0 tower temperature	SISO	344	349	353.2499
U19	D2 tower temperature	SISO	343	348	352.2499

[Type here]

Short name	Variable name	Related to	Lower bound	Nominal value	Upper bound
U20	O tower consistency	SISO	0.05	0.1	0.1425
U21	Recaust CaOH2 concentr.	SISO	3	18	30.75
U22	WL temperature	SISO	358	368	376.4999
U23	WL NaOH concentration	SISO	99.1498	100	150
U24	Steam flow 3 (digester)	FREE	0.0373	0.103	0.18025
U25	Excess WL split (digester)	FREE	0.9	1	1.07
U26	D1 water flow	FREE	68.5125	189	330.75
U27	E back-flush flow	FREE	240	484.06	847.105
U28	D2 caustic flow	FREE	0.07325	0.293	0.4797
U29	Split fraction 6 (brown stock)	FREE	0.2936	0.31915	0.3408
U30	Split fraction 8 (brown stock)	FREE	0.7176	0.78	0.83304
U31	Split fraction 9 (brown stock)	FREE	0.38	0.4	0.417
U32	Split fraction 1 (MEE)	FREE	0.7202	0.9	1.575
U33	Effect 3 steam flow	FREE	821.92	881.893	952.44
U34	Filter lower flow	FREE	0.54	0.862	1.508
U35	Kiln primary air flow	FREE	62.5	250	437.5
U36	Effect 5 exit flow	FREE	75	300	525
U37	Effect 4 exit flow	FREE	75	300	525
U38	Effect 3 exit flow	FREE	75	300	525
U39	Effect 6 exit flow	FREE	75	300	525
U40	Effect 2 exit flow	FREE	75	300	525
U41	Effect 1a exit flow	FREE	75	300	525
U42	Effect 1b exit flow	FREE	75	300	525
U43	Effect 1c exit flow	FREE	75	300	525
U44	Coolant 4 flow (post Slaker)	FREE	2.5	10	17.5

Table 2

List of the economically significant variables

Short name	Variable name	Related to	Lower bound	Nominal value	Upper bound	Costs
V1	Production rate	MPC1	629.97	629.998	630	-c_pulp
V2	Steam flow 1	SISO	0	0.175	0.398	c_dig_st
V3	Steam flow 2	MPC1	0	0.204	0.5306	c_dig_st
V4	Steam flow 4	MPC1	0	0.126	0.3172	c_dig_st
V5	Steam flow 5	MPC1	0	0.101	0.3184	c_dig_st
V6	Water flow	SISO	0	675.293	1324.6	c_water
V7	O steam flow 1	SISO	0	53.603	134	c_bl_st
V8	O steam flow 2	SISO	0	53.603	134	c_bl_st
V9	O steam flow 3	SISO	0	234.761	392	c_bl_st
V10	D1 ClO2 flow	MPC2	0	674.316	3 316	c_ClO2
V11	D1 wash water	SISO	0	6025.59	1237	c_water
V12	D1 steam flow	SISO	0	238.954	990.6	c_bl_st
V13	E caustic flow	MPC2	0	129.354	536	c_NaOH
V14	E steam flow	SISO	0	132.929	505.6	c_bl_st
V15	D2 ClO2 flow	MPC2	0	496.924	1904	c_ClO2
V16	D2 wash water	SISO	0	6164.76	6263.1	c_water
V17	Coolant flow	MPC1	0	1249.44	1264.1	c_cooling
V18	Oxygen flow	SISO	0	13.221	50	c_O2
V19	Salt-cake flow	SISO	0	56.096	168.5	cNa2 SO4
V20	Coolant 1 flow	MPC3	0	1.938	8	c_cooling
V21	Wash stream 1	SISO	0	0.041	0.1	c_cooling
V22	Fresh lime flow	SISO	0	1.848	8	c_CaO
V23	Coolant 2 flow	SISO	0	0.160	2	c_cooling
V24	Caustic flow 3	SISO	0	0.014	0.068	c_NaOH
V25	Wash stream 2	SISO	0	2.227	4.466	c_cooling
V26	Wash stream 3	SISO	0	0.683	1.508	c_cooling
V27	Wash stream 4	SISO	0	0.193	0.298	c_cooling
V28	Wash stream 4	SISO	0	0.229	0.454	c_cooling

[Type here]

Short name	Variable name	Related to	Lower bound	Nominal value	Upper bound	Costs
V29	Kiln fuel flow	MPC4	0	42.367	42.92	c_natgas
V30	Water flow	SISO	0	0.399	0.944	c_water
V31	Steam production	FREE	0	4	158.71	-c_recov
V32	Wood chips flow	MPC1	0	2.55	5.2286	c_wood
V33	O caustic flow	MPC1	0	29.000	87	c_NaOH
V34	Effect 1 steam flow	MPC3	0	942.401	1 847.2	c_steam
V35	Effect 2 steam flow	MPC4	92.36	923.600	1385.4	c_steam
V36	Steam flow 3	FREE	0	0.103	0.206	c_dig_st
V37	D1 water flow	FREE	0	189.000	378	c_water
V38	E back-flush flow	FREE	0.06	484.060	968.06	c_water
V39	D2 caustic flow	FREE	0	0.293	0.586	c_NaOH
V40	Effect 3 steam flow	FREE	0	881.893	1763.8	c_steam

Table 3

Costs and prices of the chemicals, products and utilities

Cost item	Cost (US\$/kg)
c bl st	0.0038
c CaO	0.0629
c ClO ₂	1.0000
c cooling	0.0530
c dig st	0.0065
c Na ₂ SO ₄	0.1020
c NaOH	0.2000
c nat gas	0.1702
c O ₂	0.1000
c pulp	-0.3300
c recov	-0.0051
c steam	0.0025
c water	0.0001
c wood	0.0390

3.3 Formulation of the optimization problem

The objective of the optimization in the benchmark problem is simply to maximize the profit rate from the operation of the Mill. There are two sources for revenues: the bleached pulp production and the steam production in the recovery boiler. The expenses consist of woodchips costs as the raw material, the steam, chemicals and energy costs. There are three grades of steam with different pressures used in various parts of the Pulp Mill. The bleaching chemicals are O₂, ClO₂ and NaOH. In the chemical recovery loop salt-cake, fresh lime and caustic make-up flows contribute to the costs together with the natural gas, which is used in the Lime Kiln.

In the benchmark problem, the profit of the plant given by (9) is used as the objective function for the optimization:

$$P = -(C_1V_1 + C_2V_2 + \dots + C_{40}V_{40}), \quad (9)$$

where V_i are values of the economically significant variables and C_i are their prices that are given in Table 3. Using the prices in Table 3 the profit of the Pulp Mill is about 105.9 USD/min at the nominal steady state.

3.4 Preliminary study of the process behavior

[Type here]

Some examples of the behaviour of the process are presented in the following in order to motivate the need of the iterative optimization method, as well as the quadratic static model of the process.

First let us examine the quality of the different approximations while moving the setpoint from the nominal setpoint to that obtained by the one-step optimization based on the one dimensional quadratic model. Thus those setpoints are considered which are linear combinations of the optimal setpoint and the nominal setpoint with coefficients α and $(1 - \alpha)$, correspondingly.

The simulation profit and its forecasts based on the linear and on the multidimensional quadratic models are shown in Fig. 3. The figure shows that the multidimensional quadratic approximation is much better than the linear one. However, the real profit is smooth for α over the interval $(-0.5, 0.75)$. At $\alpha = 0.75$ the behaviour of the system becomes non-smooth, thus leading to a significant increase in the errors of the forecasted at the optimal point ($\alpha = 1$). This demonstrates the effect of the control saturation in causing a non-smooth behaviour of the profit rate of the plant. The validity limits of the models constructed at the nominal setpoint are clearly shown in Fig. 3.

Fig. 3. Dependence of the real profit and its forecasts on the coefficient α

Next, an example of the non-smooth behaviour of a variable is presented. Let us consider the variations in the decision variable U23 (WL NaOH concentration) with values of +10% and +20%. The dynamics of the economically significant variables V4 and V5 (steam flows 4 and 5) are presented in Figs. 4 and 5.

It is clear from the figures that the decrease in steam 5 flow (variable V5) was stopped by the constraint. At the same time, the increase in steam 4 flow (variable V4) was also stopped. As a result, the variable V4 is a non-smooth function of the U23 decision variable, even though the constraints on V4 are inactive. In addition, variable V31 (steam production) is also a non-smooth function. This is demonstrated in Table 4.

The behaviour in the steady states of the economically significant variables with respect to the decision variables can be linear or non linear. As an example of linear behaviour, the values of the steady states of

[Type here]

economically significant variables 12 (D1 steam flow), 13 (E Caustic flow), 15 (D2 ClO₂ flow) are presented in Fig. 6 for different values of decision variable 9 (E Washer [OH]). Since the main reagent in the E tower is NaOH, decision variable 9 (E Washer [OH]) affects the rate of the reactions in the tower. The linear approximation approach gives a satisfactory approximation for such pairs of economically significant and decision variables (D1 steam flow, E Caustic flow, D2 ClO₂ flow dependence on E Washer [OH] setpoint value). However, sometimes the behavior is essentially non linear. In this case, a quadratic approximation is needed. The dependence of Economically Significant variable 9 (O steam flow 3) on decision variable 9 (EWasher [OH]) is presented, together with its quadratic and linear approximations, in Fig. 7.

Fig. 4. The steam flows 4 and 5 for a +10% variation in the 23rd decision variable

Fig. 5. The steam flows 4 and 5 for a +20% variation in the 23rd decision variable

Table 4

The dependence of some economically significant variables on variations in U_{23}

Variation of the U_{23}	Steam 4	Steam 5	Steam production
0%	-0.386	-0.2186	4148
+5%	-0.161	-0.523	4160
+10%	0.060	-0.846	4172
+15%	0.093	-1	4177
+20%	-0.073	-1	4178

In addition, some decision variables also interact strongly with each other in terms of the behaviour of the steady states of the economical significant variables (for example, seven decision variables which are used by MPC1 interact strongly with each other). Let us consider the following variations in the decision variable 1 (D2 production rate) and decision variable 8 (E kappa), and their influence on the value of economically significant variable 10 (D1 ClO₂ flow).

[Type here]

Fig. 6. Dependence of the steady states of the economically significant variables 12 (D1 steam flow), 13 (E Caustic flow), and 15 (D2 ClO₂ flow) on the decision variable 9 (E Washer [OH]) value

Fig. 7. Dependence of the steady states of the economically significant variable 9 (O steam flow 3) on the decision variable 9 (E Washer [OH]) value

According to Table 5, the mixed second derivative of ESV 10 with respect to decision variables 1 and 8 is estimated as:

$$\frac{\partial^2 V_{10}}{\partial U_1 \partial U_8} = \frac{-0.116 - 0.356 - (-0.187 - 0.298)}{0.25^2} = 0.208.$$

[Type here]

Since the number of interactions is high (there are about one hundred of significant interactions between the decision variables), the interactions cannot be ignored without losing approximation accuracy. In order to take the effect of the setpoint interactions into account, the multidimensional quadratic approximation approach has to be utilized.

It was also noted during the simulations that the upper constraint on the white liquor flow to the oxygen tower which is set at $3.77 \times 10^{-3} \text{ m}^3/\text{s}$ is often active. In fact, this flow is used by a basic control loop supervised by MPC1. In order to avoid saturation of the controller, a linear model of the white liquor flow to the oxygen tower was constructed and used by all the optimizations presented in the next section.

Table 5

Variations in decision variable 1 (D2 production rate) and decision variable 8 (E kappa)

Decision variable 1	Decision variable 8	Economically significant variable 10
Nominal	Nominal	-0.187
Nominal +25%	Nominal	-0.116
Nominal	Nominal +25%	-0.356
Nominal +25%	Nominal +25%	-0.298

4 Optimization results

4.1 Optimization based on the linear model

The optimization was carried out with both the one-step optimization method and the iteration approach described in Section 2. While the single step optimization predicts the increase in the profit rate by 26.5 USD/min against the nominal setpoint, the simulation shows only a 10.9 USD/min improvement. In fact, manipulated variable 29 (Lime Kiln fuel) is predicted by the linear model to be 40.48, but the simulated Lime Kiln fuel saturates at the upper constraint, which is 42.9. Due to saturation the process does not follow its set-point 14 (Kiln $\text{CaCO}_3\%$), which is compensated by an increase in the manipulated variable 22 (Fresh Lime flow). This leads to a significant degradation of the plant profit rate at the setpoint. Obviously, further improvement of the profit rate could be achieved with a setpoint where saturation of the Lime Kiln fuel flow is avoided. However, the bias update procedure does not take into account the effects of the control loop saturation, and is therefore not aimed at decreasing of the Lime Kiln fuel demands. In fact, after the bias update the setpoint is found, and is different from the previous one in a single component (CV37, Effect 4 exit flow). This difference does not affect the Lime Kiln, and the prediction of the Lime Kiln fuel flow remains at the upper constraint level. Finally, only an extremely small increase in the profit rate ($<0.1 \text{ USD/min}$) is achieved with the bias update.

In contrast to the single step optimization, the iterative method is able to keep the Lime Kiln fuel flow (Fig. 8), away from saturation (although it is approaching the upper constraint level). This allows an increase in the profit rate by more than 15 USD/min, which is 4 USD/min better than the single step optimization approach. While both methods give the same recommendations regarding most of the setpoints (for instance setpoints 6, 7, 9, 10, 11, 13, 15, 19, 21, 26, 27, 32, 36, 39, 40, 41, 44 are recommended to be decreased to the lowest possible level, while setpoints 2, 3, 8, 18, 24, 25, 29, 31, 33, 35, 38 to the highest possible level), the most significant difference between the setpoints is summarized in Table 6.

[Type here]

Fig. 8. Lime Kiln fuel: forecasted by the model (dashed line) and simulated (solid line)

Table 6

Comparison of the one-step and iterative optimization setpoints

Setpoint	One step method	Iterative method
V4, digester lower EA	0.72	0.58
V16, O tower temperature	-1	0.85
V20, O tower consistency	0.85	-1
V22, WL temperature	0.58	0.45
V28, D2 caustic flow	-0.75	0.64
V30, split fraction 8 (brown stock)	-0.06	0.05
V34, filter lower flow	0.06	0.26
V37, effect 4 exit flow	-0.75	0.75
V40, effect 2 exit flow	-0.75	0.75
V42, effect 1b exit flow	-0.75	0.75
V43, effect 1c exit flow	0.75	-0.75

4.2 Optimization based on the one-dimensional quadratic model

Due to the process disturbances and the fact that the steady state may not be achieved precisely, the values of the MVs can be determined only approximately with the simulations. Consequently, if one uses the set of variations with steps of +5% and -5% (that were used for the linear model identification) from the nominal values of the decision variables, the errors of the second derivatives estimations will be too large (although these variations allow relatively accurate estimations of the first derivatives). This is the reason why the simulations with variations of +25% and -25% from the nominal values of the decision variables have been used in order to compute the second derivative matrix L . There are only a few exceptions to this rule: the smaller variations of decision variables U23 (WNaOH concentration), U25 (Excess WL split), U29 (Split fraction 6), and U32 (Split fraction 1), are used because their 25% variations violate the constraints and destabilize the plant. Matrix L is presented in Fig. 9 in a graphical form.

The dots mark the elements of matrix L with absolute values more than 0.1. The economically significant variable V31 (steam production), and the decision variables U23 (WL NaOH concentration) and U25 (Excess WL split), are scaled in a manner which produces a large number of significant second derivatives. However, the main conclusion from Fig. 8 is that some decision variables (such as U1 (D2 production rate), U2 (Digester kappa), U3 (Digester upper EA), U4 (Digester lower EA), U7 (O kappa), U8 (E kappa), U32

[Type here]

(Split fraction 1 MEE), U33 (Effect 3 steam flow)) have responses of at least several economically significant variables that cannot be described satisfactorily with the linear approximation only.

Fig. 9. Matrix of the second derivatives of the economically significant variables with respect to the decision variables

In addition, 83 elements of matrix L are also larger than 0.1 (taking into account the sign of the chemical costs), and only 45 elements are smaller than -0.1 (taking into account the sign of the chemical costs). As a result, the number of positive second derivatives is almost twice the number of negative ones. Since the positive second derivatives increase the values of the economically significant variables in comparison to the linear approximation, the linear approximations forecasted, on the average, too low levels for the economically significant variables and, as a consequence, it predicts too large an increase in the Pulp Mill profit.

Optimization was carried out with both one-step optimization method and the iteration approach. While both methods give the same recommendations for most of the setpoints (for instance setpoints 7, 10, 11, 13, 19, 21, 26, 27, 33 are recommended to be decreased to the lowest possible level while setpoints 8, 12, 18, 20, 24, 25, 29, 30, 35 increased to the highest possible level), the most significant difference between the setpoints is summarized in [Table 7](#).

For the one step solution the approximations promises an increase of 18.0 USD/min in the profit rate against the nominal steady state while, at the same time, the simulation shows only a 13.6 USD/min increase. In fact, saturation of the white liquor flow to the oxygen tower takes place at the level $3.77 \times 10^{-3} \text{ m}^3/\text{s}$, although the flow was predicted by the model at the level $2.73 \times 10^{-3} \text{ m}^3/\text{s}$. As the result, because insufficient delignification takes place in the oxygen tower, the Cl_2O flow to D1 tower following the oxygen tower must be increased. After the bias update, the model promises an increase of 16.0 USD/min, but the simulation shows about 13.5 USD/min. Basically, in the bias update procedure nothing is changed in order to avoid saturation of the white liquor flow to the oxygen tower.

[Type here]

Table 7

Comparison of the one-step and the iterative optimization setpoints

Setpoint	One step method	Iterative method
U2, digester kappa	1	0.94
U3, digester upper EA	0.45	0.42
U4, digester lower EA	0.42	0.40
U15, digester liquor temperature	-1	-0.61
U16, O tower temperature	-1	0.65
U22, WL temperature	0.84	0.49
U28, D2 caustic flow	-0.75	-0.59
U32, split fraction 1 (MEE)	-0.13	0
U34, filter lower flow	-0.05	0.08
U40, effect 2 exit flow	-0.18	-0.07
U43, effect 1c exit flow	0	0.74

For the iterative method, the dynamics of the forecasted and the simulated white liquor flow to the oxygen tower are shown in Fig. 10. A comparison of the white liquor flows to the oxygen tower against the results obtained by the single step optimization is presented in Fig. 11. The figure demonstrates the sufficiency of the control capacities for the iterative optimization setpoint (although the steady state value of the flow is at the upper constraint level). The quadratic model predicts about the same level of Cl_2O flow to the D1 tower for both setpoints. However, due to insufficient delignification in the oxygen tower, the Cl_2O flow must be significantly increased in the simulation at the setpoint derived by the single step optimization. This increase is demonstrated in Fig. 12. The economical losses related to the increase in consumption of expensive Cl_2O are estimated as about 1.4 USD/min.

Fig. 10. White liquor flow to the oxygen tower: forecasted by the model (dashed line) and simulated (solid line)

Fig. 11. White liquor flow to the oxygen tower, comparison of the single step and iterative optimization results

[Type here]

Fig. 12. Cl_2O flow to the D_1 tower, comparison of the single step and iterative optimization results.

As a result, the iterative method is able to achieve an improvement of 14.3 USD/min in the profit rate against the nominal setpoint, which is a slightly better (0.7 USD/min) result compared to the one step method, even though both optimizations are based on the same quadratic model. The dynamics of the predicted and the simulated profit rate improvement against the nominal steady state are presented in Fig. 13.

Fig. 13. Iterative optimization profit rate improvement forecasted by the model (dashed line) and simulated (solid line)

4.3 Multi dimensional quadratic approach

Finally, both one-step optimization and the iterative optimization were performed with the multidimensional quadratic model. While both methods give the same recommendations for most of the setpoints (for instance setpoints 7, 9, 10, 11, 13, 15, 19, 20, 21, 26, 27, 28, 31, 33, 36, 37, 38, 39, 40, 41, 42, 43, 44 are recommended to be decreased to the lowest possible level while setpoints 8, 12, 24, 25, 29, 30, 35 increased to the highest possible level), the most significant difference between the setpoints is summarized in Table 8.

[Type here]

Table 8

Comparison of the one-step and iterative optimization setpoints

Setpoint	One step method	Iterative method
U2, digester kappa	0.75	0.54
U3, digester upper EA	0.36	0.33
U4, digester lower EA	0.27	0.31
U16, O tower temperature	-0.04	-0.77
U18, E0 tower temperature	0.38	0.20
U22, WL temperature	0.62	0.42

For the one step solution the approximations promises an increase of 17.7 USD/min in the profit rate against the nominal steady state while, at the same time, the simulation shows only a 15.6 USD/min increase. In general, the multidimensional quadratic model appears to be accurate, and the re-estimation of the bias at this setpoint does not change it very much. Thus, after the bias update, the improvement in the profit rate still remains at the same level of 15.6 USD/min. Although saturation of the white liquor flow to the oxygen tower appears after the bias update procedure, it does not have any significant economical effect.

For the iterative method, the dynamics of the forecasted and the simulated profit rate improvement are shown in Fig. 14. As the result, the iterative method is able to achieve an improvement of 15.8 USD/min in the profit rate compared to the nominal setpoint, which is almost the same result that was achieved by the single step optimization. In fact, both the iterative and the single-step optimizations achieve similar results, since there is no significant saturation of the control capacities at the setpoint derived by the single-step optimization.

Fig. 14. Iterative optimization profit rate improvement forecasted by the model (dashed line) and simulated (solid line)

5 Conclusions

Optimization of the steady state economic efficiency of an industrial process must take into account the fact that the decision variables of the optimization (setpoints of the control system) affect the process through the control strategy. The saturation effects of control system on the steady state of the manipulated variables of the process was briefly studied in the paper, and it was concluded that the finite difference estimation of the objective gradient does not provide correct results in the presence of active manipulated variables constraints. As a result, the necessary optimality conditions cannot usually be checked directly and a static model of the process must therefore be employed to evaluate the approximated optimality conditions

[Type here]

introduced in the paper. In fact, the approximated optimality conditions are the most accurate approximation of the original optimality conditions that can feasibly be checked.

The gradient-based optimization methods were not used in this study due to problems with the gradient estimation and the impossibility of evaluating the optimality conditions without a static model of the process. An iterative optimization method was proposed that keeps the iterations within the area free of control saturation where the static model of the process is valid. The presented method was able to find a solution satisfying the approximated optimality conditions.

The performance of the approximated optimality conditions depends on the accuracy of the static plant model employed by the optimization. Thus three different static plant models were constructed and used to perform both one step and iterative optimization. The multidimensional quadratic model was of satisfactory quality during the optimizations. However, if it is suspected that all the proposed models are not of the proper quality, then the model can be completely re-estimated after a certain number of steps of the iterative method. Since the iterative method keeps all the manipulated variables away from their limits, it is possible to perform some variations in the setpoint without saturation of the control system capacities.

The paper presents two examples of degradation of the economic efficiency at the setpoints derived by the single step optimization due to saturation of the control system capacities. The first example is related to limitations on the Lime Kiln fuel flow, while the second example presents the case of saturation of the white liquor flow to the oxygen tower. In both cases, the iterative optimization method was able to avoid saturation, and it also demonstrated the better performance compared to that of the single step optimization method using the same static plant model.

Acknowledgements

The authors would like to express their gratitude to the professor Francis Doyle, who granted the Pulp Mill Benchmark Model software.

References

- Castro, J. J., & Doyle, F. J. (2004). A pulp mill benchmark problem for control: Problem description. *Journal of Process Control*, 14, 17–29.
- Klugman, S., Karlsson, M., & Moshfegh, B. (2007). A Scandinavian chemical woodpulp mill. Part 1. Energy audit aiming at efficiency measures. *Applied Energy*, 84, 326–339.
- Luyben, W. (1989). *Process modeling, simulation and control for chemical engineers* (2nd ed.). New York: McGraw-Hill.
- Mercangöz, M., & Doyle, F. J. (2008). Real-time optimization of the pulp mill benchmark problem. *Computer and Chemical Engineering*, 32, 789–804.
- McDonough, T. J., Uno, S., Rudie, A. W., & Courchene, C. E. (2008). Optimization of ECF bleaching of Kraft pulp. *TAPPI Journal*, 7(1), 4–10.
- Santos, A., & Dourado, A. (1999). Global optimization of energy and production in process industries: A genetic algorithm application. *Control Engineering Practice*, 7(4), 549–554.
- Sarimveis, H. K., Angelou, A. S., Retsina, T. R., Rutherford, S. R., & Bafas, G. V. (2003). Optimal energy management in pulp and paper mills. *Energy Conversion and Management*, 44, 1707–1718.
- Savulescu, L. E., & Alva-Argaez, A. (2008). Direct heat transfer considerations for improving energy efficiency in pulp and paper Kraft mills. *Energy*, 33, 1562–1571.
- Sidrak, Y. (1995). Model-based optimization of Kamyr digester operation. *TAPPI Journal*, 78(3), 93–98.
- Smith, I., Christlmeier, F., & Van Winkle, R. (1986). Optimization of recovery boiler control. *Pulp and Paper Canada*, 87(3), 125–128.

[Type here]

- Tang, W., Wang, M., He, L., & Itoh, H. (2007). Neural network based double-objective optimization and application to pulp washing process improvement. *Industrial and Engineering Chemistry Research*, 46(14), 5015–5020.
- Thibault, J., Taylor, D., Yanofsky, C., Lanouette, R., Fonteix, C., & Zaras, K. (2003). Multicriteria optimization of a high yield pulping process with rough sets. *Chemical Engineering Science*, 58, 203–213.
- Westerlund, T., Hammar, T., Löfman, N., Karjaluoto, J., Åström, L., & Haglund, T. (1986). Optimization of the lime feed in a recausticizing plant. *Paper and Timber*, 68(11), 828–836.