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DYNAMIC OPTIMIZATION OF A FCC CONVERTER UNIT: NUMERICAL ANALYSIS

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Abstract - Fluidized-bed Catalytic Cracking (FCC) is a process subject to frequent variations in the operating conditions (including feed quality and feed rate). The production objectives usually are the maximization of LPG and gasoline production. This fact makes the FCC converter unit an excellent opportunity for real-time optimization. The present work aims to apply a dynamic optimization in an industrial FCC converter unit, using a mechanistic dynamic model, and to carry out a numerical analysis of the solution procedure. A simultaneous approach was used to discretize the system of differential-algebraic equations and the resulting large-scale NLP problem was solved using the IPOPT solver. This study also does a short comparison between the results obtained by a potential dynamic real-time optimization (DRTO) against a possible steady-state real-time optimization (RTO) application. The results demonstrate that the application of dynamic real-time optimization of a FCC converter unit can bring significant benefits in production.
Keywords: Dynamic Optimization; FCC Converter Unit; Dynamic Optimization; DRTO; RTO.

INTRODUCTION

The Fluidized-bed Catalytic Cracking Unit (FCCU) is one of the most profitable process units of a petroleum refinery, since it transforms low-value raw-materials into commercial products of high-aggregated value.

The FCC reaction section, known as the converter, is a flexible equipment, and can generate high yields of LPG (liquefied petroleum gas) if suitable operating conditions are used. On the other hand, it is also capable of maximizing the yields of cracked naphtha or LCO (light cycle oil) when the market prices of motor gasoline or diesel fuel are favorable. Due to its high profitability, FCC units usually operate at maximum capacity, which means maximum feed rate and maximum power applied to the gas compressor and air blower drivers.

There are frequent transitions in the operating point of a FCC converter caused by changes in the feed quality. Such changes are due to variations in the raw-material quality or in the recipes of the different streams blended to compose the feed (coker gasoil, naphtha, or atmospheric residue). Changes can also happen due to the pursuit of higher profitability, which may demand the displacement of LCO fractions into gasoline or gasoline fractions into LPG. Environmental conditions and limitations of the equipment capacities in other process areas also disturb the operation of a FCC unit.

These facts suggest that Dynamic Real-Time Optimization (DRTO) is an interesting alternative to optimize such units, which are subject to frequent changes in the process operating conditions and production objectives. Despite this, technical literature cites only the use of steady-state Real-Time

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Optimization (RTO) systems in industrial units.

There are two classes of real-time applications that use dynamic optimization algorithms. The first class is MPC - Model Predictive Control (Zavala, 2008; Zavala et al., 2008) - and the second is DRTO (Kadam et al., 2002; Kadam et al., 2003). It is important to distinguish these two kinds of applications. The MPC has a fixed objective function, a final time and an execution frequency. All future control actions are calculated every execution cycle, but only the first action of each control variable is actually implemented in the process. The nonlinear formulation (NMPC) is usually applied to continuous chemical processes with complex behavior and frequent grade transitions (Tlacuahuac et al., 2005). On the other hand, in DRTO applications the objective function is defined according to the problem to be solved and all control actions are implemented in the process as reference trajectories to the advanced control layer. The optimization of recipes of batch or semi-batch processes is a usual candidate for the use of DRTO, which is executed by triggering. The trigger is a mechanism that monitors the process and verifies whether any changes related to the dynamic optimization problem structure or important disturbances have occurred (Kadam et al., 2003). If this is the case, the DRTO system triggers the optimizer in order to obtain a new optimal recipe; otherwise the DRTO system simply downloads and executes the last valid optimal recipe calculated by the optimizer. Continuous processes with frequent operating-points or grade transitions that demand a cyclic execution time also provide great opportunities for DRTO.

The MPC, RTO and DRTO systems use the well-known measurement-based optimization technique. This method deals with uncertainties caused by changes in initial conditions, model mismatch (uncertain model parameters) and process disturbances (Kadam et al., 2007). There are two common schemes that can be adopted for real-time application problems (Srinivasan and Bonvin, 2007). The first one is the explicit scheme where the algorithm performs the state estimation (with measurement validation, data reconciliation, model parameters updating and state estimation), dynamic optimization and control action implementation (with results analysis, recipe scheduling procedure and command implementation). This scheme is usually adopted in MPC, RTO and DRTO applications. The second scheme that can be used is the implicit method, widely known as NCO-Tracking (Necessary Conditions of Optimality), which exploits the switching structure of the optimization problem (Srinivasan et al., 2003) and uses the measurements to directly adapt input trajectories. This is also known as on-line re-optimization via feedback and is very adequate for solving large-scale problems, which are very expensive in terms of CPU effort, since there is no need of solving the dynamic optimization problem in real time (Srinivasan and Bonvin, 2007). This kind of application has a triggering system that monitors the process and starts the dynamic optimizer every time the optimization problem structure changes or a significant disturbance invalidates the solution obtained by the self-optimizer controller.

There are uncertainties on the optimizer solution caused by model fidelity (i.e., model parameters uncertainty), noises and errors in the measurement sensors (Forbes and Marlin, 1996). Due to the fact that not all optimizer solutions should be implemented, it is necessary to analyze the results and decide when the optimizer recipe should be implemented in the plant operation. Miletic and Marlin (1996 and 1998) proposed a method for RTO results analysis based on the measurement of variability and its effect on the optimizer solution. The results analysis hypothesis test would be performed every RTO run in order to discriminate noises and errors in the measurements from model parameter changes.

The core of a DRTO system consists of the solution of a dynamic optimization problem in the continuous time domain, represented by a Differential Algebraic Optimization Problem (DAOP), where the process model is written in the form of DAE (Differential-Algebraic Equations). Consistent initial conditions are provided by state estimators based on process measurements feedback.

The dynamic optimization problems are usually solved by direct methods, which transform the DAOP into a NLP problem using control vector parameterization. The first significant initiatives for solving the DAOP using direct methods are due to Pollard and Sargent (1970), and Sargent and Sullivan (1977). They used piecewise constant control profiles to integrate the DAE model and solve the resulting NLP problem sequentially (single shooting), also called feasible path methods, because they produce feasible states trajectories from the suggested control profiles. In the early 80's, the limitations of the single-shooting method were well known and the researchers had been experimenting with several possibilities for solving DAOP. In 1984, Bock and Plitt presented the multiple-shooting method where the control profiles are discretized, the time horizon is divided into time intervals, and the states trajectories are obtained by integration in each interval with guessed initial conditions. In the same year, Biegler (1984) applied quadrature with orthogonal collocation in finite elements on DAE systems using piecewise constant control parameterization. This study practically inaugurated the use of simultaneous methods for solving DAOP, where all variables (control, state, and algebraic) are discretized. This method is also called infeasible path because the state trajectories are assured to be feasible only at the solution of the optimization problem. The multiple-shooting method is an intermediary approach between simultaneous and sequential methods.

The control and optimization of FCC converters has already been the subject of many studies. Optimization of this process has been made through MPC (Odloak et al. 1995) and steady-state RTO (Chitnis and Corropio 1998; Zanin et al., 2000a). NMPC has also been applied (Ali and Elnashaie, 1997) as well as other RTO strategies, such as optimization in the same layer as advanced control (Odloak et al., 2002; Gouvêa and Odloak, 1998). Zanin et al. (2000b) made a comparative study of the use of different optimization strategies in FCC converters.

This study has three main objectives: (1) To show the viability of solving dynamic optimization problems for a real industrial case, consisting of a complex system represented by a large process model; (2) To study the discretization methodology applied to the dynamic system in the optimization problem, where the effects of the number of finite elements, collocation points and element grouping are analyzed in terms of quality of the results and real-time applicability; (3) To make a short comparison between DRTO and RTO results in order to arouse interest for DRTO applications in industrial plants optimization.

FCC PROCESS DESCRIPTION

The FCC conversion section comprises the feed pre-heating furnace, the reactor-regenerator system, the air blower, the main fractionating tower, and the gas compressor. The cracking process uses a high-temperature tubular reactor to catalytically break chemical bonds and transform heavy molecules into smaller ones, thus producing fuel gas, LPG, cracked naphtha (gasoline), LCO, decanted oil and, as a side product, coke. The coke, which is produced by condensation and dehydrogenation reactions, deposits onto the catalyst surface, resulting in its deactivation. Therefore, catalyst regeneration is mandatory and this process generates a lot of energy, which is used to heat the feed up to the cracking reaction temperature.

The FCC converter model used in this work, developed by Secchi et al. (2001), is constituted of the following parts: riser model, separator model, gas compressor model, regenerator model, and valves and controllers models. These models describe a FCC UOP stacked converter, Figure 1, used by PETROBRAS in the Alberto Pasqualini refinery (REFAP S/A). The model was adjusted to the operating conditions of this particular process unit and was found to describe its dynamic behavior fairly well. Additional information about the model can be found in Fernandes et al. (2008) and Santos (2000).

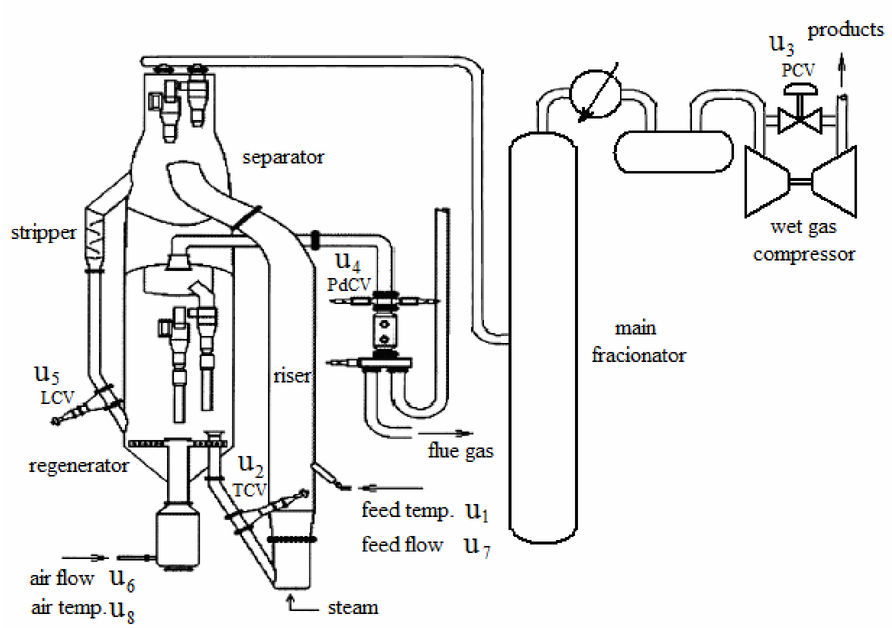

Figure 1: FCC UOP Stacked Converter (Secchi et al., 2001).

Riser Model

The Riser is modeled as an adiabatic plug flow reactor, with the kinetics described by the ten lumps model of Jacob et al. (1976) and using catalyst deactivation and coke formation tendency functions.

The dynamic model of the riser is represented by the mass balance for each lump and coke, using the reaction kinetics for each species and the energy balance. The resulting partial differential equations were discretized using the backward finite-difference technique, with a log-scale non-uniform mesh of 20 points, a number that was found to be satisfactory.

Separator Model

The separator is assumed to be a continuous stirred tank, which separates the catalyst from the vapor products (hydrocarbons). The model of this equipment (based on mass and energy balances) focuses on the prediction of the catalyst level in the separator, the coke content in the spent catalyst, and the catalyst temperature. The pressure dynamics is established by a momentum balance.

Gas Compressor Model

The gas compressor is modeled as a single stage centrifugal compressor, running at constant speed. The polytrophic flow model predicts the compressor suction pressure and, consequently, defines the pressure in the main fractionating tower and in the separator. A recycle stream around the compressor controls the suction pressure and the mass balance is given by assumed dynamics.

Regenerator Model

The catalyst regeneration is carried out by burning the coke deposited in the catalyst in a fluidized-bed reactor. This bed is modeled as emulsion and bubble phases that exchange mass and heat. The bubble phase is assumed to be at the pseudo steady-state condition. The disengagement section is modeled as two serial continuous well-mixed tank reactors, corresponding to the diluted and flue gas phases, according to Figure 2.

The regeneration kinetics assume that the coke combustion reactions occur in the emulsion, diluted, and gas phases. Component mass balances for O_2, CO, CO_2, H_2O, and coke describe the dynamic behavior of these reactions, resulting in five state equations for each phase of the regenerator. The catalyst inventory in the regenerator is modeled by an overall mass balance. The pressure behavior in the regenerator is obtained through the global mass balance in the gas phase. An energy balance applied to each phase predicts the dynamic behavior of the temperatures in the regenerator. Considering that the catalyst loss in the regenerator is negligible, the total mass of catalyst that enters the regenerator is accumulated or sent to the riser. The coke in this catalyst is mainly burned in the emulsion phase, but it also suffers reaction in the diluted and gas phases.

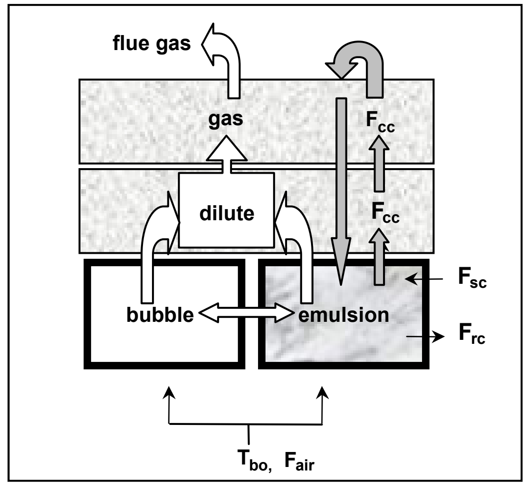

Figure 2: Regenerator phases (Secchi et al., 2001).

Valves and Controllers Models

Four degrees of freedom provide stability to this type of FCC converter. These degrees of freedom are eliminated by placing regulatory PI controllers in the following positions:

- Compressor suction pressure controller, using a control valve (PCV) in the compressor recycle stream;
- Reaction temperature controller, using a control valve (TCV) in the stand-pipe to the riser;
- Pressure drop controller between the reactor and the regenerator, using a control valve (PdCV) in the orifice chamber of the regenerator flue gas;
- Catalyst level controller in the separator, using a control valve (LCV) in the stand-pipe to the regenerator;

The dynamics of the valve openings are determined by their respective time constants. Additionally, each PI controller has one state equation to describe the integral action. The reaction temperature control was performed by the dynamic optimizer, via supervisory action directly on the slide-valve. Therefore, only three PI controllers were used.

Empirical Correlations for Product Yields

The FCC converter model does not directly supply information like product yields and conversion, which are necessary to analyse and optimize the process. In the present case, empirical correlations are used to provide such information, i.e., the volumetric conversion and the yields of fuel gas, LPG, gasoline (GLN), light cycle oil (LCO), decanted oil (OCLA), and coke (CK).

The optimization problem has 8 control variables (Figure 1). In the reaction section, there are the variables related to the feed of the unit: feed flow rate (u_7) and feed temperature (u_1). In order to control the reaction temperature, the slide valve (TCV) opening (u_2) is manipulated to adjust the catalyst flow to the riser. The rectification and catalyst inventory are controlled by manipulating the level control valve - LCV (u_5). The pressure control of the system is performed through the manipulation of the regenerator-reactor differential pressure control valves, PdCV (u_4), and pressure control of the compressor suction, PCV (u_3). The air flow rate and air temperature (u_6 and u_8) are manipulated to control the coke burning and, thus, the catalyst regeneration.

The FCC converter model has hundreds of dependent variables. The main variables are related to the control of the reaction, regeneration, and system pressure. The reaction and regeneration temperatures, products yields, and the resulting overall profit are the most important variables to be monitored.

FORMULATION OF DYNAMIC OPTIMIZATION PROBLEM

The dynamic optimization problem of a process has the following general form:

$$\min_{z(t),y(t),u(t),t_f,p} \varphi\left(z\left(t_f\right),y\left(t_f\right)\right) \tag{1}$$

subject to:

Dynamic Model (ODE):

$$F\left(\frac{dz(t)}{dt},z(t),y(t),u(t)\right)=0 \tag{2}$$

Algebraic Equations (AE):

$$G\left(z(t),y(t),u(t)\right)=0 \tag{3}$$

Initial Conditions:

$$z(0)=z^0 \tag{4}$$

Bounds:

$$\begin{aligned} & z^L \le z(t) \le z^U \\ & y^L \le y(t) \le y^U \\ & u^L \le u(t) \le u^U \end{aligned} \tag{5}$$

where z(t) is the vector of differential state variables, y(t) is the vector of algebraic variables, u(t) is the vector of control variables and t_f is the final time on the optimization problem.

Solution of the Dynamic Optimization Problem

The infinite dimension dynamic optimization problem can be solved through variational methods, using Pontryagin's maximum principle and solving the resultant two-point boundary value problem (TPBVP), or by approximating to a finite formulation, with predefined functional forms for the control variables. In this last case, the resultant nonlinear programming (NLP) problem can be solved by sequential, multi-shooting or simultaneous approaches. In the sequential approach, only the control variables are discretized or parameterized, while in the simultaneous approach the whole system is discretized in the time domain, usually using orthogonal collocation techniques. See the work of Biegler et al. (2002) for a more detailed review of these methods.

In this work the simultaneous strategy has been used, where the continuous problem is converted into a NLP problem when approximating the state and control profiles by a family of orthogonal polynomials on finite elements (Cervantes, 1998). In this procedure, the DAE system is converted into a system of algebraic equations, whose residues are exactly satisfied at the collocation points. As we can see in Figure 3, the Radau collocation on finite elements is used to discretize the system.

This collocation is equivalent to the implicit Runge-Kutta method and its precision depends on the number and the location of the collocation points and the integration step (Tanartkit and Biegler, 1995; Logsdon and Biegler, 1989). In practice, the number of collocation points is usually small, because high-degree polynomials tend to present oscillatory behavior.

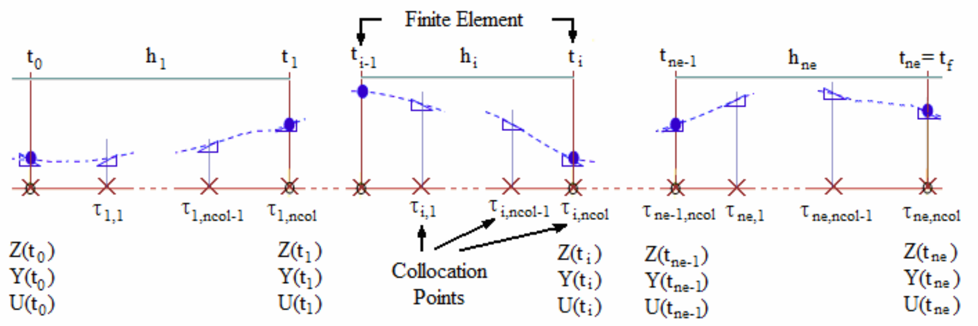

Figure 3: Collocation on finite elements.

The application of the finite elements method allows the partition of the prediction horizon into a finite number of subintervals necessary to guarantee the solution accuracy when low-degree polynomials are used. The sizes of the finite elements affect the stability and accuracy of the results (Tanartkit and Biegler, 1995) and they are also related to the dimension of the optimization problem (total number of decision variables). Using the finite elements method, the continuity of the state variables should be guaranteed along the whole time horizon. On the other hand, the algebraic variables may be discontinuous at the element boundaries, because the control variables can be allowed to present discontinuities at these points.

In general, the usage of large-scale NLP algorithms in the simultaneous approach is more robust and workable for solving discretized DAE systems. However, difficulties to solve the problem may arise if the finite element locations are manually chosen. In particular, inconsistent linearization of the constraints may occur in places where there are non-smooth nonlinearities and the NLP algorithm fails to converge.

To calculate the values of z, y and u at any time t, the following interpolating polynomials can be used (Lang and Biegler, 2007; Lang et al., 1999). For the state variables the approximation results in:

$$z(t) = z_{i-1} + h\sum_{q=1}^{ncol}\Omega_q\left(\frac{t-t_{i-1}}{h_i}\right)\frac{dz}{dt_{i,q}} \tag{6}$$

where z_{i-1} is the value of the differential variable at the beginning of element i, $dz/dt_{i,q}$ is the value of its time derivative in element i at the collocation point q, $h_i = (t_i - t_{i-1})$ is the length of element i, and Ω_q is a polynomial of order ncol.

The control profiles and algebraic variables are approximated in a similar way and the equation takes the following form:

$$y(t) = \sum_{q=1}^{ncol}\Psi_q\left(\frac{t-t_{i-1}}{h_i}\right)y_{i,q} \tag{7}$$

$$u(t) = \sum_{q=1}^{ncol}\Psi_q\left(\frac{t-t_{i-1}}{h_i}\right)u_{i,q} \tag{8}$$

where $y_{i,q}$ and $u_{i,q}$ are the values of the algebraic and control variables, respectively, in element i at collocation point q and Ψ_q is a Lagrange polynomial of order ncol. The values of $\Omega_q(\tau)$ and $\Psi_q(\tau)$ are obtained by the following polynomials:

$$\Omega_q(\tau) = \sum_{j=1}^{ncol}\frac{c_{ncol+1-j,q}\tau^j}{j!} \tag{9}$$

$$\Psi_q(\tau) = \sum_{j=1}^{ncol}\frac{c_{ncol+1-j,q}\tau^{(j-1)}}{(j-1)!} \tag{10}$$

where $c_{ncol+1-j}$ are coefficients of the polynomials and τ is the dimensionless time inside each finite element. The algebraic and control variables are evaluated using interpolator polynomials with one order lower than the polynomials used to evaluate the state variables (Ψ_q is the derivative of Ω_q). This is made to allow the discontinuities at the element boundaries (Cervantes, 1998).

After the discretization of the DAE system, the optimization problem can be rewritten as the following NLP problem (Tanartkit and Biegler, 1997; Lang et al., 1999):

$$\min_{u(t)}\varphi(z(t_f), y(t_f)) \tag{11}$$

Subject to:

Discretized DAE model (residues at collocation points):

$$F\left(z_{i-1},\dot{z}_{ij},y_{ij},u_{ij}\right)=0 \quad (12)$$

$$G\left(z_{i-1},\dot{z}_{ij},y_{ij},u_{ij}\right)=0 \quad (13)$$

for $i=1,\cdots,ne;\ j=1,\cdots,ncol$

Continuity equation:

$$z_i = z_{i-1} + h_i \sum_{q=1}^{ncol} \Omega_q(1)\,\dot{z}_{iq} \quad (14)$$

for $i=1,\cdots,ne$

Initial Conditions:

$$z(0)=z^0 \quad (15)$$

Bounds:

$$\begin{aligned} & z^L \le z_{ij}, z_i \le z^U \\ & y^L \le y_{ij} \le y^U \\ & u^L \le u_{ij} \le u^U \end{aligned} \quad (16)$$

for $i=1,\cdots,ne;\ j=1,\cdots,ncol$

where F is the discretized DAE system, G are the discretized algebraic constraints, t_{ij} is the collocation point j in element i, and $\Omega_q(1)$ is a polynomial evaluated at the end of the element.

Element Grouping for Control

In order to reach the necessary accuracy for the discretized variable, sometimes it is necessary to increase the number of finite elements. As a consequence, the control variable trajectories can present undesired discontinuities. This can be problematic for applications in real time, because a small step interval should be avoided at this level of control actions. In industrial plants, it is usual to maintain the control variables constant for a larger time interval. To solve this problem, the alternative is the use of elements grouping for control (EGFC), available in the software DynoPC (Lang and Biegler, 2007). This feature is similar to the grouping strategy used in predictive controllers in order to better distribute the control actions along the prediction horizon.

The element grouping consists of keeping the control variables constant along all elements contained in each group, as shown in Figure 4 (Lang and Biegler, 2007). The number of elements per group should be compatible with the operation actions. Still there is the freedom to put as many finite elements as necessary to obtain the desired accuracy of the discretized state and algebraic variables without increasing the number of decision variables in the optimization problem.

Usually, in dynamic optimization problems the number of control variables is small and the number of state variables is very large. In this case the rSQP algorithm (reduced SQP) is efficient (Waanders et al., 2002). The solution of these problems is also efficient using the interior point algorithms; however, they require improvements and many of them have been proposed. The following ones can be highlighted: the use of the preconditioned conjugated gradient method (PCG) to update the control variables (Cervantes and Biegler, 2001); and the introduction of a filter in the strategy of the line search, where the objective function competes with the infeasibility of the problem (Wächter, 2001).

In the interior point algorithm the original NLP problem can be written as:

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & c(x)=0 \\ & x \ge 0 \end{aligned} \quad (17)$$

where f(x) is the objective function and c(x) are the equality constraints.

The barrier function is added to reduce the dimension of the problem, which then takes the form:

$$\begin{aligned} \min \quad & \varphi_\mu(x) = f(x) - \mu \sum_{i=1}^{n} \ln(x_i) \\ \text{s.t.} \quad & c(x)=0 \end{aligned} \quad (18)$$

where μ is the barrier parameter and n is the number of inequality constraints.

All of these features were implemented in the IPOPT algorithm developed by Carnegie Mellon University (CAPD Report, 2003).

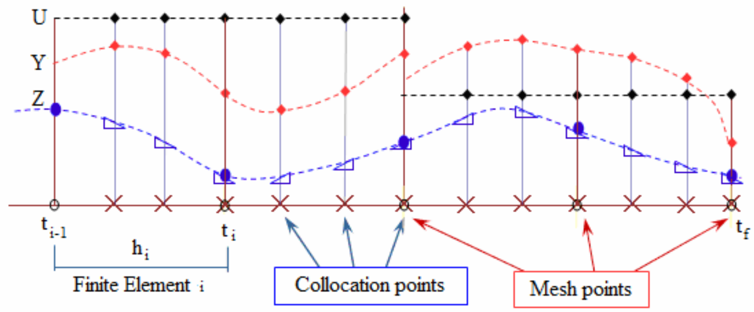

Figure 4: Element Grouping for Control (Lang and Biegler, 2007).

Configuration of the Objective Function

In the optimization of FCC converters there are some concurrent production objectives. The maximization of the operational profit is a common objective; however, due to the optimization of the refinery supply chain, there are moments where some specific products need to be maximized. There are situations where the local optimum of an isolated process unit is not the global optimum of the supply chain. In order to attend these situations, single or multiple objectives can be adopted. In this dynamic optimization problem, the integral of different factors along a day (t_f = 24 h) were maximized. The most common objectives are presented on Table 1.

Table 1: Common production objectives in FCC converter optimization

Case	Production Objective	Objective Function	Additional Constraints
1	Maximum operational_profit	$FObj_1 = -\int_0^{t_f} Profit.dt$ (19)	$Profit \geq Profit_{min}$ (20)
2	Maximum total_conversion	$FObj_2 = -\dfrac{\int_0^{t_f} Conv_v V_{Feed}.dt}{\int_0^{t_f} V_{Feed}.dt}$ (21)	$Conv_v \geq Conv_{min}$ (22)
3	Maximum feed throughput	$FObj_3 = -\int_0^{t_f} V_{Feed} dt$ (23)	$V_{Feed}^{min} \leq V_{Feed} \leq V_{Feed}^{max}$ (24)
4	Maximum LPG Production	$FObj_4 = -\int_0^{t_f} \dfrac{\eta_{LPG}}{100} V_{Feed} dt$ (25)	$V_{LPG}^{min} \leq \dfrac{\eta_{LPG}}{100} V_{Feed} \leq V_{LPG}^{max}$ (26)
5	Maximum Gasoline (GLN) Production	$FObj_5 = -\int_0^{t_f} \dfrac{\eta_{GLN}}{100} V_{Feed} dt$ (27)	$V_{GLN}^{min} \leq \dfrac{\eta_{GLN}}{100} V_{Feed} \leq V_{GLN}^{max}$ (28)
6	Maximum LCO Production	$FObj_6 = -\int_0^{t_f} \dfrac{\eta_{LCO}}{100} V_{Feed} dt$ (29)	$V_{LCO}^{min} \leq \dfrac{\eta_{LCO}}{100} V_{Feed} \leq V_{LCO}^{max}$ (30)

where

$$\text{Profit} = \text{Revenue} - \text{Costs} \tag{31}$$

$$\text{Revenue} = m_{FG}\, Pr_{FG} + m_{CK}\, Pr_{CK} + V_{LPG}\, Pr_{LPG} + V_{GLN}\, Pr_{GLN} + V_{LCO}\, Pr_{LCO} + V_{OCLA}\, Pr_{OCLA} \tag{32}$$

$$\text{Costs} = V_{Feed}\, Pr_{Feed} + m_{Cat}\, Pr_{Cat} + Q_{PreH}\, Pr_Q + Q_{Proc}\, Pr_{Fuel} + Pot_{Blwr} C_{Blwr} + Pot_{Compr} C_{Compr} \tag{33}$$

The notation used is the following: m_i is the mass flow rate of stream i, V_i is the volumetric flow rate, and Pr_i is the price. The subscript FG is flue gas to the boiler, CK is coke produced by the catalyst. LPG is liquefied petroleum gas, GLN is gasoline, LCO is the light cycle oil, OCLA is the clarified oil produced in the main fractionator column, Feed is the riser feed stream, Cat is catalyst, Q is the fuel used in the pre-heating system, and Fuel is the fuel used in the process unit. Q_{PreH} is the heat duty of the pre-heating system and Q_{Proc} is the energy consumed in the process unit. Pot_{Bwr} and C_{Bwr} are the power and the operation cost of the air blower and Pot_{Compr} and C_{Compr} are the power and the operation cost of the FCC gas compressor. Notice that this objective function is not monotonic because there are positive terms (Revenue) and negative ones (Costs). For the second objective, Conv means the volumetric conversion in FCC. Note that the variable η in the objectives 4 to 6 is the yield for the specified stream.

Multi-Objective Function Formulation

In the general case, each production objective can be represented in the following way:

$$FObj_i = -\int_0^{t_f} OBJ_i . dt \tag{34}$$

The multi-objectives problem can be written as a weighted sum of each specific objective:

$$\varphi = \sum_{i=1}^{n} k_i FObj_i \tag{35}$$

where k_i is the weight of each specific objective and n is the number of concurrent objectives.

The integral in each specific objective is obtained by differentiating the original objective function and creating a new state, φ, which can be added to the set of differential equations. Therefore, the objective function assumes the following form:

$$\frac{d\varphi}{dt} = -\sum_{i=1}^{n} k_i\, Obj_i \; ; \; \varphi(0) = 0 \tag{36}$$

The specific production objectives are mutually exclusive. One can maximize the production of any specific stream by setting the other objectives to zero.

Additional Constraints

Besides the constraints usually imposed on the states and the control variables, supplementary constraints were added to represent bounds in the production objectives in order to satisfy the requirements defined by the scheduling people in the refinery. These additional constraints are presented in the last column of Table 1. Usually the LPG and GLN markets are greater than the process unit capacity and, consequently, the planner and scheduler frequently (for simplicity) decide for FCC production maximization. The common operational instruction that represents this objective is the maximization of feed throughput, which is the easiest to be implemented in the process unit. All case studies presented in this paper focused on this production objective (<u>feed throughput</u>, case 3 in Table 1).

CASE STUDIES AND RESULTS

The dynamic optimization problem has been solved by applying the IPOPT algorithm embedded in the DynoPC dynamic optimization software developed at Carnegie Mellon University (Lang and Biegler, 2007).

This chapter comprises three parts: the first one consists of studying the influences of the main discretization parameters on the solution of the optimization problem. The second part uses the best tuning of the discretization procedure for the solution of a dynamic optimization problem. The third part presents a comparison between solutions obtained by RTO and by DRTO.

The dynamic optimization of a FCC converter is a large-scale and complex problem. Usually, in the open literature, studies about solutions of dynamic optimization problems have been presented for small/medium scale problems sizes or large-scale problems with simple models. In this article, we show the ability of DynoPC to deal with large complex problems, which cannot be considered an easy task.

The dimension of the continuous problem is related to the size of the dynamic model, as presented in Table 2.

Table 2: Size of the dynamic model

Number of variables	Qty
No. of Differential variables	274
No. of Algebraic variables	21
No. of Control variables	8
No. of Parameters	124

When using DynoPC (with full discretization strategy), it is necessary to bound all variables of the problem. The initial conditions and bounds of the differential variables are shown in Table 3.

The model of the FCC riser was discretized into 20 elements, having 12 state variables in each element with initial conditions and variable bounds presented in Table 4.

The initial conditions and bounds of the algebraic variables are shown in Table 5.

The initial values and bounds of the control variables are shown in Table 6.

In the first part of this study, the effects of the number of finite elements (ne), number of collocation points (ncol), and number of finite elements groups were analyzed as in the following.

Table 3: Bounds and initial conditions of state differential variables of FCC converter

Differential Variable	Description	Lower bound	Initial value	Upper bound
Z(1)	Separator Height	20	25.8	30
Z(2)	Coke on spent catalyst	0	0.0105	0.05
Z(3)	Separator temperature	0.3	0.755	1
Z(4)	Coke on regenerated catalyst	0	0.0041	0.005
Z(5)	Emulsion temperature	0.3	0.972	1.5
Z(6)	O_2 in the emulsion	0	0.0059	0.01
Z(7)	CO in the emulsion	0	0.126	0.2
Z(8)	CO_2 in the emulsion	0	0.245	0.5
Z(9)	Coke in the diluted phase	0	0.0041	0.01
Z(10)	O_2 in the diluted phase	0	0.0024	0.005
Z(11)	CO in the diluted phase	0	0.048	0.4
Z(12)	CO_2 in the diluted phase	0	0.105	0.5
Z(13)	Diluted phase temperature	0.3	0.96	1.5
Z(14)	Coke in the dense phase	0	0.0041	0.01
Z(15)	O_2 in the dense phase	0	0.0011	0.003
Z(16)	CO in the dense phase	0	0.048	0.4
Z(17)	CO_2 in the dense phase	0	0.105	0.5
Z(18)	Dense phase temperature	0.3	0.96	1.5
Z(19)	Regenerator Pressure	1	3.28	5
Z(20)	Riser Pressure	1	2.96	5
Z(21)	Wet gas compressor suction pressure	0.2	0.8900	3
Z(22)	Actual TC valve position	0	0.515	1
Z(23)	Actual LC valve position	0	0.2532	1
Z(24)	Actual PdC valve position	0	0.3159	1
Z(25)	Actual PC valve position	0	0.3344	1
Z(26)	Error in separator level controller	-100	0	100
Z(27)	Error in regen.-sep. diff. pressure controller	-10	0	10
Z(28)	Error Wet gas compr. Suc. Pressure controller	-10	0	10
Z(29)	Integral of the profit	0	0	1
Z(30)	Integral of the feed rate	0	0	1
Z(31)	Integral of the conversion	0	0	1
Z(32)	Integral of LPG production	0	0	1
Z(33)	Integral of Gasoline production	0	0	1
Z(34)	Integral of LCO production	0	0	1

Table 4: Bounds and initial conditions of state differential variables on riser discrete elements of FCC converter

Differential variable			Description	Lower bound	Initial value	Upper bound
Z(35)	…	Z(263)	Temperature in the riser element i	0.30	0.79	1.50
Z(36)	…	Z(264)	Paraffins in the light oil in the riser element i	0	0.0125	0.1000
Z(37)	…	Z(265)	Naphtenes in the light oil in the riser element i	0	0.0063	0.01
Z(38)	…	Z(266)	Aromatics in the light oil in the riser element i	0	0.0001	0.0010
Z(39)	…	Z(267)	Catalyst in the light oil in the riser element i	0	0.00042	0.001
Z(40)	…	Z(268)	Paraffins in the heavy oil in the riser element i	0	0.49	1.00
Z(41)	…	Z(269)	Naphtenes in the heavy oil in the riser element i	0	0.26	1.00
Z(42)	…	Z(270)	Aromatics in the heavy oil in the riser element i	0	0.0076	0.01
Z(43)	…	Z(271)	Catalyst in the heavy oil in the riser element i	0	0.0046	0.01
Z(44)	…	Z(272)	Gasoline in the riser element i	0	0.048	0.100
Z(45)	…	Z(273)	Coke and Gas in the riser element i	0	0.16	0.50
Z(46)	…	Z(274)	Coke in the riser element i	0	0.0095	0.0500

Table 5: Bounds and initial conditions of the algebraic variables of FCC converter

Algebraic variable	Description	Lower bound	Initial value	Upper bound
Y(1)	Reaction Temperature	530.0	535.5	540.0
Y(2)	Emulsion temperature	360.3	720.7	1081.0
Y(3)	Diluted phase temperature	354.9	709.8	1064.7
Y(4)	Dense phase temperature	353.8	707.5	1061.3
Y(5)	Inlet riser temperature	279.6	559.2	838.8
Y(6)	Wet gas compressor suction pressure	0.445	0.890	1.335
Y(7)	Regenerator-separator differential pressure	0.002	0.240	0.5
Y(8)	TCV differential pressure	0.0001	0.205	0.5
Y(9)	Wet gas compressor power	0	14.14	30
Y(10)	Regenerated catalyst flow rate	0	14.82	30
Y(11)	Separator height level	10	22.58	40
Y(12)	Regenerator height level	20	61.89	100
Y(13)	Mass conversion	0	0.792	1
Y(14)	Gasoline yield	0	0.463	1
Y(15)	LCO yield	0	0.094	1
Y(16)	Clarified oil yield	0	0.114	1
Y(17)	Wet gas yield	0	0.310	1
Y(18)	Coke on regenerated catalyst	0	0.003	1
Y(19)	Coke production	0	0.055	1
Y(20)	LPG yield	0	0.300	1
Y(21)	Total mass conversion	0	0.800	1

Table 6: Bounds and initial values of the control variables of the FCC converter

Control variable	Description	Lower bound	Initial value	Upper bound
U(1)	Air flow rate	50	77.3	120
U(2)	TCV set value	0	0.515	1
U(3)	Feed flow rate	1000	3500	5000
U(4)	Feed temperature	200	330	400
U(5)	Separator level control set point	10	22	40
U(6)	Regenerator-Separator DP control set point	0	0.3159	1
U(7)	Separator height level control set point	0	0.9	1
U(8)	Wet gas compressor suction pressure set point	100	165	200

Influence of the Finite Elements Grouping on the Solution of the Optimization Problem

The main objective of the grouping is to minimize the number of changes in the plant along the optimization horizon, without losing the discretization accuracy. Besides that, reducing the problem dimension also decreases the computational effort. We used 1, 3, 6, and 10 groups, with equally distributed elements, in order to show the effects of the choice of the number of element groups on the optimization results. Piecewise constant functions control the variables profiles, that is, within each element or group of elements the control variables remain constant. The discretization was carried out using 40 finite elements and 3 collocation points in each element. It is observed that, above 6 groups, the results of the optimizer are not very different from each other (Figs. 5 to 7). This means that the operation can plan a control action every 4 hours without compromising the solution of the optimization problem. Frequent disturbances (e.g., periods of less than four hours) are uncommon in real FCC plants and this work also considers that there are no un-modeled disturbances in the process operation.

It can be noted in Figure 8 that the objective function practically reaches its maximum value with 6 groups and that the grouping of elements reduces the degrees of freedom of the problem and, consequently, results in a sub-optimal solution. In the present case, this sub-optimal solution is evidenced by a lower throughput.

In addition, Figures 9 and 10 show that the CPU time increases with the number of groups, presenting a quasi-linear behavior when expressed in CPU time per iteration (Fig. 10). In this particular optimization problem, we observed an increase of 7.5% of CPU time per iteration. If the benefit in the objective function is not significant, there is no motivation to increase the number of element groups. The verified total execution time of about 45 minutes is applicable in the real-time case (about 3% of optimization horizon – 24 hours) because the optimal recipe is scheduled and downloaded to the plant once each time. If the problem structure does not change and no disturbance appears, it is not necessary to review the optimal solution before the final time of the problem. If there are frequent changes in the process operation, this execution time is still acceptable for a one-hour re-optimization cycle. Moreover, it is possible to reduce the CPU time by executing the optimization using parallel processing for function evaluation and linear algebra steps that consume 80% of the total CPU time.

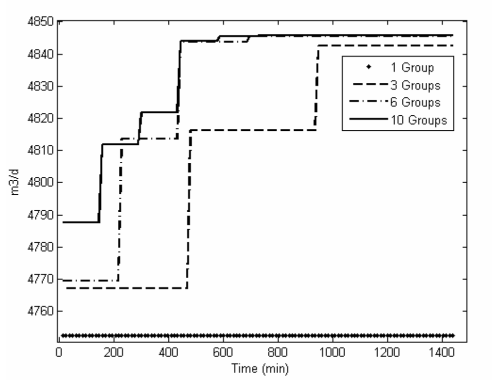

Figure 5: Feed flow rate.

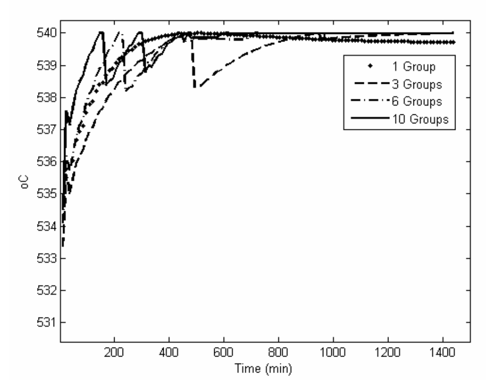

Figure 6: Outlet Riser Temperature (Reaction).

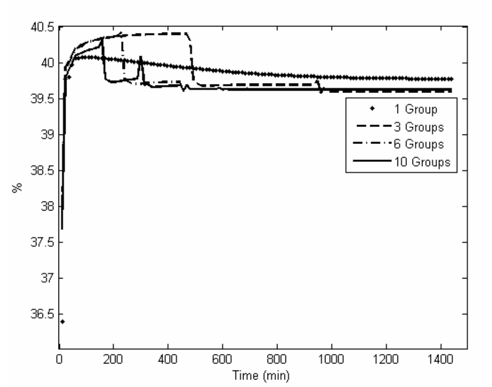

Figure 7: Gasoline yield.

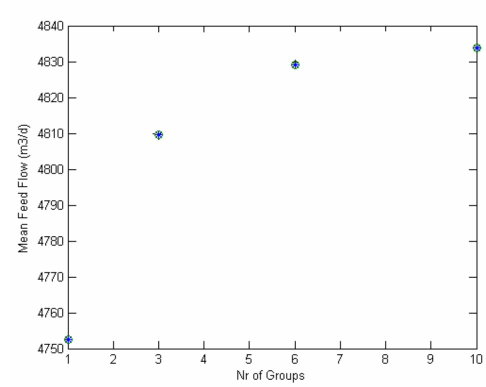

Figure 8: Objective function values – case max. feed throughput.

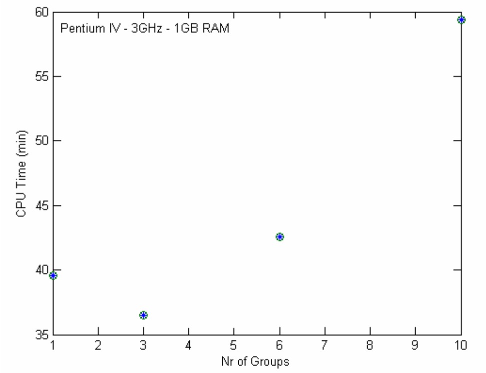

Figure 9: CPU time spent in IPOPT and function evaluations.

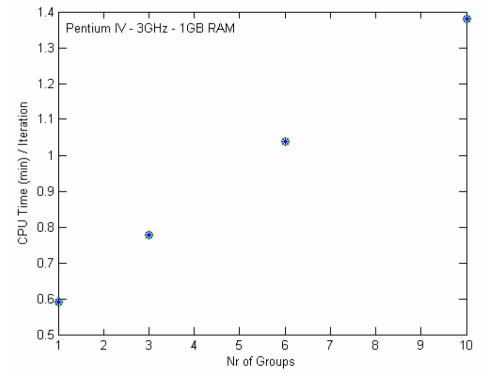

Figure 10: CPU time per iteration spent in IPOPT and function evaluations per iteration.

Influence of the Number of Finite Elements on the Solution of the Optimization Problem

This section analyzes the effect of the number of finite elements on the discretization quality. The sizes of the elements represent the integration steps and reducing these sizes or increasing the number of finite elements will increase the discretized model accuracy and stability.

In order to demonstrate the effect of the number of elements on the discretization quality, 20 and 40 finite elements were used in the case of 10 element groups and 3 collocation points. The 10 groups were used because the focus of the analysis was to verify the accuracy of the results and not the computational performance.

The loss of accuracy was not significant when using 20 elements, as can be observed by the similar trajectories of the control variables shown in Fig. 11 for the feed flow rate. Discontinuities slightly higher in the derivatives can be observed in the reaction temperature (Fig. 12) and gasoline yield (Fig. 13) trajectories when using 20 elements, showing less accuracy in the discretized model than 40 elements.

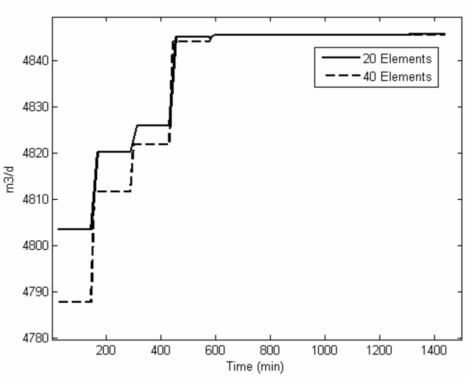

Figure 11: Feed flow rate

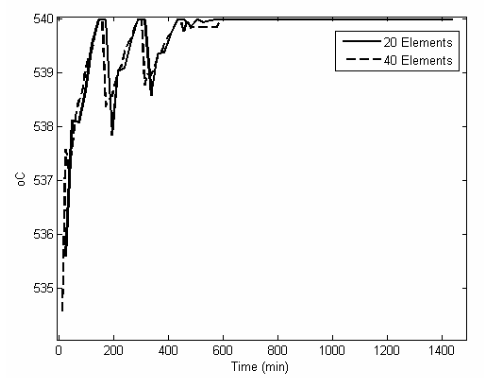

Figure 12: Outlet Riser Temperature (Reaction).

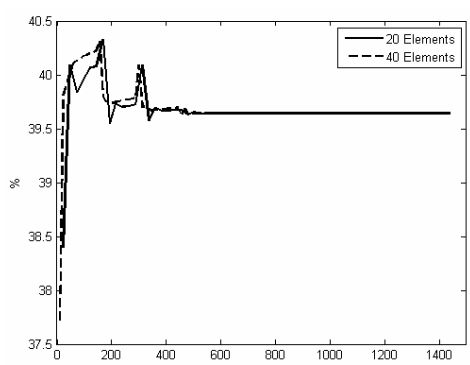

Figure 13: Gasoline yield.

Influence of the Number of Collocation Points on the Solution of the Optimization Problem

In this section, the effect of the number of collocation points on the discretization quality was analyzed. The number and locations of the collocation points also affect the discrete model accuracy and the solution stability of the optimization problem. These aspects are related to the order of the Runge-Kutta method. The number of collocation points is usually small (high-degree polynomials tend to produce oscillatory solutions). In this case, 2 and 3 collocation points with 20 and 40 finite elements and 10 element groups were used in the comparative analysis.

It can be noted that defining 20 finite elements and 2 collocation points resulted in a poor discretization. This can be observed in the quality of the optimization solution (Fig. 14) and in the differential and algebraic variable trajectories (Figs. 15 and 16) when compared with the most accurate solution (40 elements and 3 collocation points). It can also be noted that, by adding one collocation point (ne = 20 and ncol = 3), the quality of the discretization was significantly improved. On the other hand, when increasing the number of finite elements instead of the number of collocation points (ne = 40 and ncol = 2), the improvement in the discretization quality was not as good as when increasing the number of collocation points. In this case, the problem size (total number of discrete points) is bigger than the case ne = 20 and ncol = 3, requiring more computational time.

Therefore, it can be concluded that the discretization quality of the system is more sensitive to the increase in the number of collocation points than the increase in the number of finite elements. This is because increasing the number of collocation points results in an increase in the integration order, while increasing the number of elements decreases the integration step, the first effect being much more significant. In the case studied, it is possible to say that the discretization with 20 elements, 3 collocation points, and 6 groups provided the necessary accuracy with low computational cost to solve the real-time optimization problem.

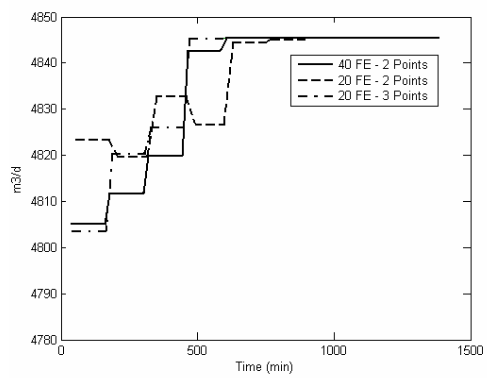

Figure 14: Feed flow rate.

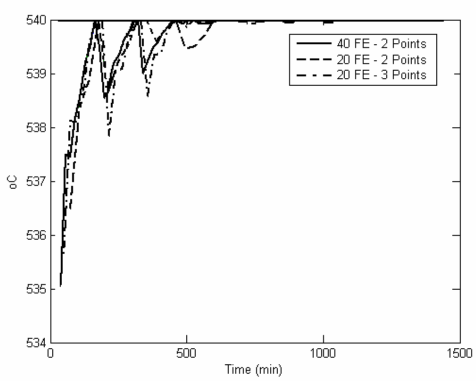

Figure 15: Outlet Riser Temperature (Reaction).

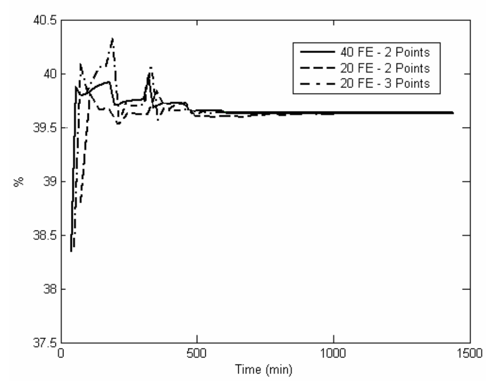

Figure 16: Gasoline yield.

Regarding the full discretization parameters, the number of both finite elements and collocation points affects the solution accuracy of the optimization problem. This accuracy is affected more by the number of collocation points than by the number of finite elements. In both cases, there is a compromise between the solution accuracy and the computational effort required to solve the optimization problem. If the computational effort is a limiting factor in enabling the use of DRTO system, then we should reduce the number of finite elements (the solution accuracy is less sensitive to this parameter). It is required to choose carefully the number of finite elements and their sizes in order to obtain an accurate optimum solution, because an inappropriate choice may limit the control variables manipulations, leading the plant to a sub-optimal condition. It may be preferable to use parallel computing techniques to improve computational performance than reducing the number of elements in the problem. Furthermore, it is important to remember that the number of collocation points is related to the order of the equivalent Runge-Kutta method. A high number of collocation points may cause oscillations on the optimum solution and even lose the optimizer solution stability. It seems that a good value is the use of three collocation points.

Considering the element grouping, the goal is to reduce the amount of disturbance in the process and to avoid the possibility of constraints violation. It is important to remember that the solution of the discretized problem may not guarantee that the constraints will be respected outside the collocation point (discrete points). When the elements are grouped, some intermediate discrete points are included between two successive control movements. Moreover, element grouping (smaller number of groups) reduces the computational effort for solving the optimization problem. This element grouping does not affect the problem solution accuracy, but reduces the degrees of freedom imposed on the optimizer. Therefore, the obtained solution is sub-optimal. It is also important to consider the existence of an optimal number of groups where the objective function values are slightly changed. This number is a problem-dependent parameter and its optimal value must be found for the studied case.

Nominal Solution of the Case Study – Maximum Feed Throughput

After tuning the optimizer, we present the nominal solution of the FCC converter dynamic optimization. In this work, the “Maximum Feed Throughput” case was selected, because this is the most frequent specific production objective of the FCC converter unit. According to the problem definition described above, the number of variables involved in the problem is given in Table 7. We used 40 finite elements, 3 collocation points and 10 groups in this case study in order to explore the optimization in large dimension problems. The dimension of the NLP problem resulting from the discretization of the DAOP is considered to be a large-scale optimization problem (system with 47642 variables). This fact turns this case an interesting problem to validate the use of this kind of optimization technique for solving large and complex optimization problems.

Table 7: Number of variables in the formulation.

Number of differential variables (nz)	274
Number of algebraic variables (ny)	21
Number of control variables (nu)	8
Number of finites elements (ne)	40
Number of collocation points/element (ncol)	3
Total number of discretized variables	47642
Total number of constraints	47594
Total number of lower bounds	14440
Total number of upper bounds	14440

The maximization of feed throughput is prioritized when it is necessary to use the whole capacity of the process unit. In this case, the limits of catalyst circulation or rotating machines (air blower and/or gas compressor) are reached. Notice that the optimizer increased the feed flow rate, opened the catalyst valve to the maximum, dropped the suction pressure of the gas compressor, and reduced the pressure drop between the reactor and regenerator (Figs. 17 to 20). In order to supply the additional energy demanded by the system, the regenerator and riser temperatures were increased (Figs. 21 and 22).

As a result of the dynamic optimization, the feed rate changed from 3500 m^3/d to 4845 m^3/d. It can also be observed that there was an increase of volumetric conversion (Fig. 23). The gasoline yield was increased and LCO yield decreased. Note that the decanted oil yield (OCLA) almost did not change (Fig. 24). The optimizer increased the yield of the more valuable product and, as a consequence, the operational profit was increased by the order of 5.5 thousand dollars a day ($0.20/bbl). This is in the range of the normal potential of benefit of advanced control and RTO applications.

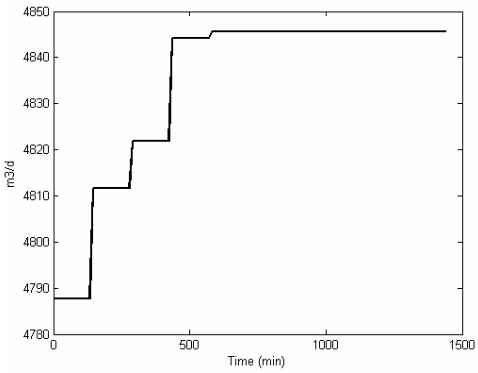

Figure 17: Feed flow rate.

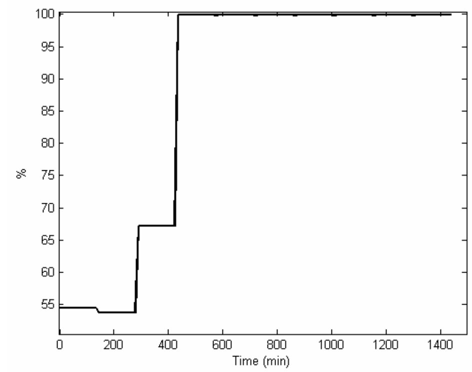

Figure 18: TCV control signal.

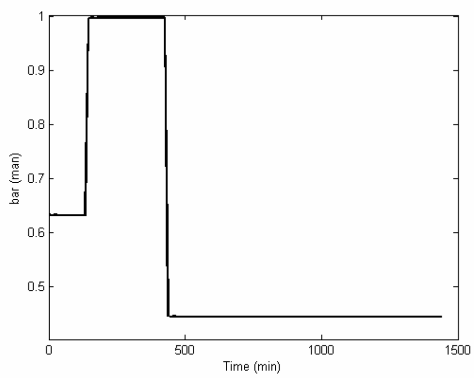

Figure 19: Suction pressure of gas compressor.

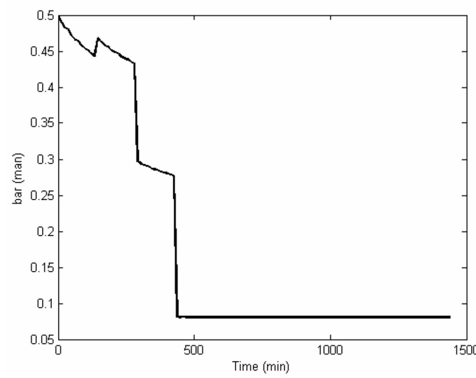

Figure 20: Differential pressure between reactor and regenerator.

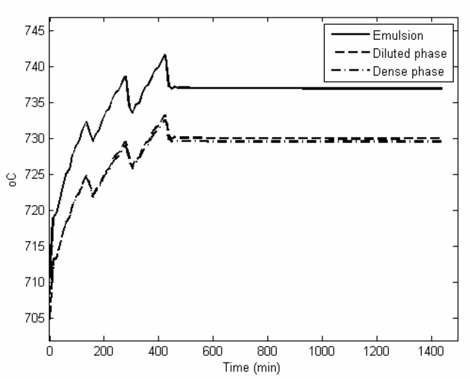

Figure 21: Regenerator's temperatures.

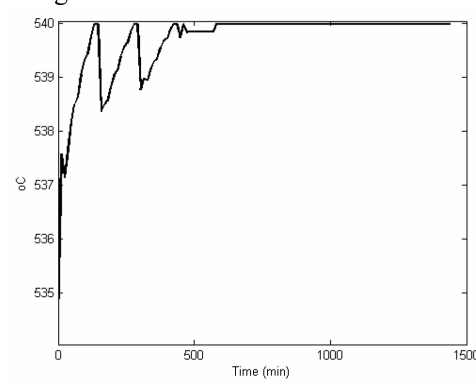

Figure 22: Riser temperature (reaction).

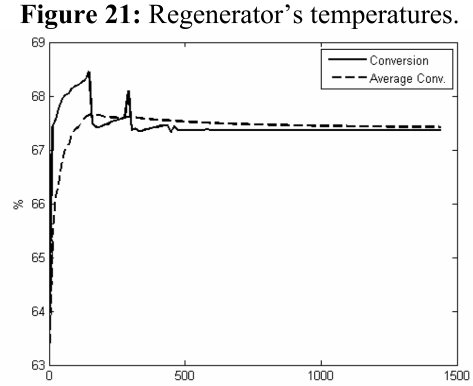

Figure 23: Volumetric conversion.

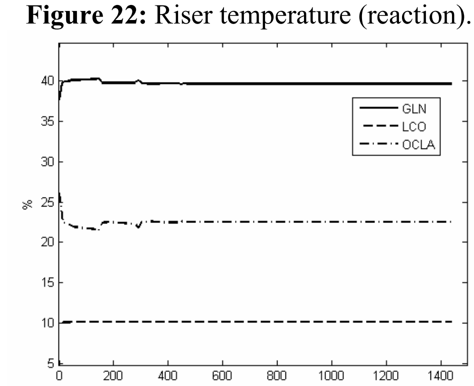

Figure 24: Volumetric yields (GLN – gasoline, LCO – light oil of recycle, OCLA – decanted oil).

Comparison Between DRTO and RTO Solutions

In this section, we make a short comparison between results obtained by RTO and DRTO systems. Usually, RTO system run together with MPC by downloading the optimal control position (called ideal resting value) or some optimal bounds for the constraints (Zanin et al., 2002; Odloak, 2009), while DRTO can be directly integrated with MPC or DCS systems (Kadam et al., 2003). In this case study, we simulated the RTO solution integrated with a MPC system by imposing path constraints to the optimizer. This strategy means that the RTO solution will not violate the MPC constraints (Tables 5 and 6) during the plant operation. The main premise of this study is the absence of important disturbances or changes in the problem structure during the operation. This fact allows us to suppose that the solutions obtained by RTO and DRTO systems will not change during the optimization horizon (i.e., it is not necessary to re-optimize during this period). In the real case, the RTO usually runs every 2-4 hours and the DRTO will run when the optimizer monitor triggers the optimization module.

Based on a specific scenario, the RTO system computes only one optimal operating point, where the decision variables are optimized in the steady-state position. On the other hand, the DRTO system optimizes the whole path of the process operation. Based on these characteristics, it is expected that some differences in the optimizers' results will arise.

Considering case 3 – maximum feed throughput, both optimizers solved the same optimization problem structure, but in different ways. In order to maximize the feed rate, the optimizers usually maximize the use of the air blower, minimize the wet gas compressor suction pressures and maximize the catalyst circulation. As consequence, the process is pushed to the maximum reaction temperature constraint. Both optimizers used the same air flow rate in the blower at maximum value (120 ton/h). Another important control variable is the suction pressure of the gas compressor. This pressure should be minimized in order to maximize the throughput in the FCC unit. Figure 25 shows that both RTO and DRTO systems minimized this pressure, but the DRTO system used a different profile when reducing the riser temperature (Fig. 26), while the RTO set this pressure to its lower bound, preventing the MPC to follow a more favorable path. In the choice of this operation strategy, the DRTO optimizer found a solution where more feed can be pushed into the FCC unit. Figure 27 shows this difference, and it can be noted that it was possible to reach a feed flow rate of 4752.56 m^3/d using RTO and 4833.91 m^3/d when optimizing with DRTO. Note also that the DRTO system proposes process set point changes (manipulations) each 2-4 hours. The RTO suggested a higher feed temperature (Figure 28) due to the lower catalyst circulation into the reactor and lower reaction temperature (Figure 29). The mean conversion (67.72% - RTO and 67.44% - DRTO) and the gasoline yields (39.85% - RTO and 39.69% - DRTO) were slightly higher in the RTO case (Figures 30 and 31). However, the DRTO solution seems to be better than the one generated by RTO, because the feed flow rate in the DRTO case is 81.35 m^3/d higher than in the RTO case and the total gasoline production (1894.3 m^3/d - RTO and 1918.6 m^3/d - DRTO) is 24.3 m^3/d higher than in the RTO case. The recipe suggested by the RTO is different from the optimal policy recommended by the DRTO due to the fact the riser temperature reached the maximum 4 times in the time interval 0 – 600 min in the latter (Figure 29). Note that the DRTO changed the suction pressure of the gas compressor (Figure 25) and feed temperature (Figure 28) in order to avoid the riser temperature constraint violation (Figure 29) and to reduce the feed flow rate (Figure 27). The RTO solution had no opportunity to do that because the solution is an optimal operating point and it needs to be more conservative to avoid this constraint violation.

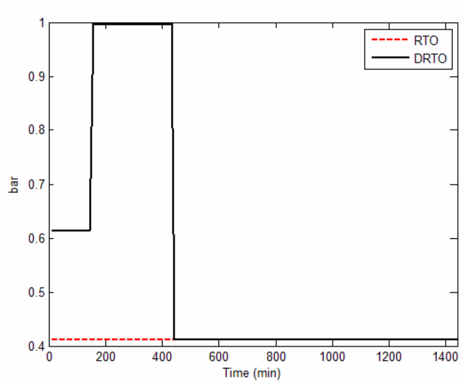

Figure 25: Suction pressure of gas compressor.

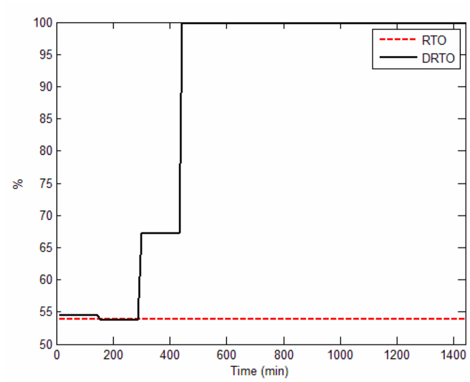

Figure 26: TCV control signal.

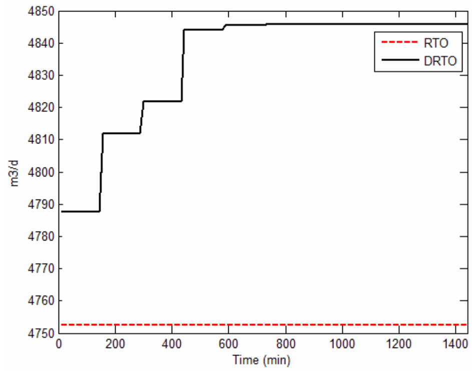

Figure 27: Feed flow rate

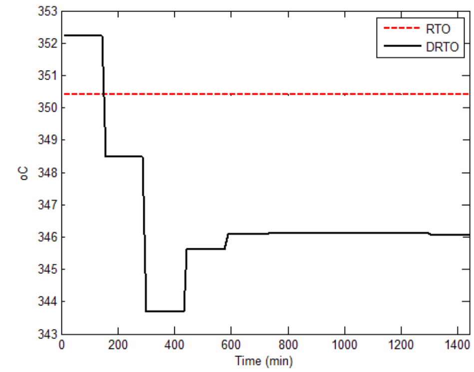

Figure 28: Feed temperature at the riser entrance

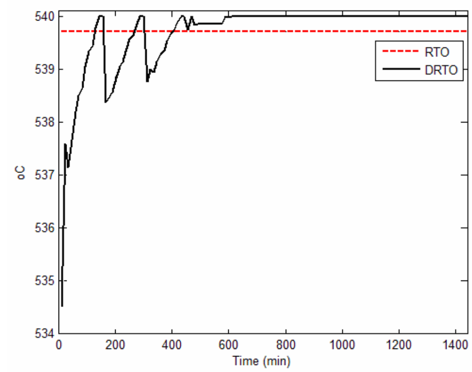

Figure 29: Outlet Riser Temperature (Reaction)

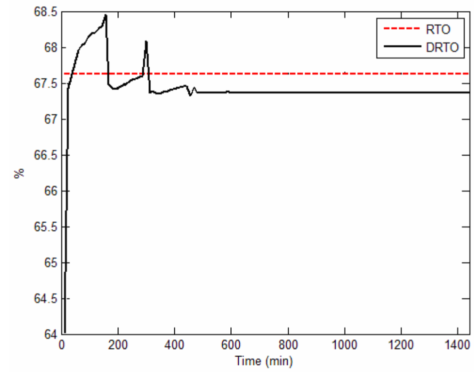

Figure 30: Volumetric reactor conversion.

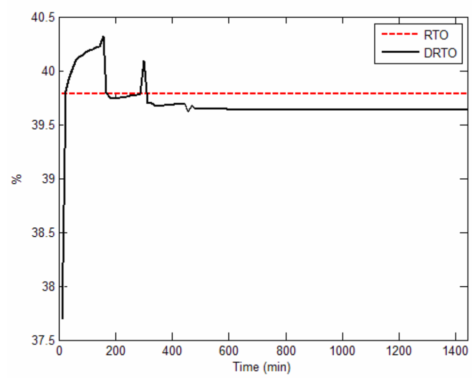

Figure 31: Volumetric gasoline yield.

In this work, we simulate a situation where the RTO system was integrated with MPC application. This was made by including path constraints of a one-step dynamic optimization problem. This has been done by using the same structure problem of the DRTO optimizer, which is equivalent to using a RTO with the best possible MPC solution (with the same constraints and objective function used by the equivalent DRTO system). The main difference of using this approach from the real plant situation is due to the fact the MPC does not solve the same DRTO problem. The MPC objectives are the minimization of the distances between the values of control variables and their ideal values at rest (IRV) suggested by the RTO. If the NMPC solves the same DRTO problem, it will not be necessary to use RTO or DRTO in the upper optimization level. We are not discussing here about the alternative of using the NCO-tracking approach, but we are supposing the adoption of traditional MPC that are used in real plant applications. Furthermore, the optimal solution suggested by the RTO application may lead the MPC to violate some path constraints. Consequently, the MPC may obtain an infeasible solution, deteriorating the optimizer solution (not reaching the target) or violating some soft constraints along its trajectory.

Another important difference between the uses of RTO vs. DRTO is related to the application of operating recipes. In the DRTO case, these recipes are usually included in the optimization problem, whereas the RTO only perceives recipe changes after they appear in the plant. In the later case, there is a time interval where the plant operates in a non-optimized way by violating some constraints or even seeking a wrong optimal point.

CONCLUSIONS

Regarding the sensitivity analysis of the discretization parameters (number of finite elements, number of collocation points and number of groups of elements), this work has shown the importance of the adequate choice of these parameters to improve the solution quality and to reduce the computational cost. The results demonstrate that an inadequate choice of the number of collocation points and the number of finite elements can compromise the discretization quality of the model or the computational effort to solve the optimization problem. It was also observed that the quality of the discretization is more sensitive to the increase of the number of collocation points than the number of finite elements. This is due to the fact that increasing the integration order is more effective than the reduction of the integration step.

This study has also shown the importance of criteria for grouping finite elements for control. It is essential to discover the minimum number of groups necessary to find an acceptable optimal solution. A small number of groups can interfere in the maximum potential to be reached by the optimizer due to the lack of degrees of freedom in the control variables. On the other hand, a large number of groups can have high computational cost and may generate undesired movements in the plant.

Additionally this study leads one to conclude that the solution of dynamic optimization problems with high complexity and high dimension is not an easy task. Despite this, it is possible to obtain good solutions for industrial cases since, although computational performance for solving the dynamic optimization problem is limited, it is acceptable for the real case studied and the CPU time performance can still be improved by using parallel computing strategies.

The dynamic optimization of the FCC converter generated results coherent with what is expected in an industrial unit. The results demonstrate that the application of DRTO in this kind of unit can bring slightly more benefits when compared with the traditional RTO solution. The simultaneous approach has been shown to be effective for the solution of the problem, but it demanded a lot of time to tune the discretization parameters of the control variables. The strategy of grouping intervals for the control variables was the one that presented better performance.

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REFERENCES

Ali, E. E. and Elnashaie, S. S. E. H., Non-linear Model Predictive Control of Industrial type IV Fluid Catalytic Cracking (FCC) units for maximum gasoline yield. Ind. Eng. Chem. Res., 36, 389-1007 (1997).

Biegler, L. T., Cervantes, A. M. and Wächter, A., Advances in Simultaneous Strategies for Dynamic Process Optimization. Chem. Engng. Sc., 57, 575-593 (2002).

CAPD Report, Center for Advanced Process Decision-Making. CAPD Report. March. (2003).

Cervantes, A. and Biegler, L. T., Large-Scale DEA Optimization Using a Simultaneous NLP Formulation. AIChE, J., 44, (5), 1038-1050 (1998).

Cervantes, A. and Biegler, L. T., Optimization Strategies for Dynamic Systems. Encyclopedia of Optimization. Kluwer, 4, 216-227 (2001).

Chitnis, U. K. and Corropio, A. B., On-line optimization of a Model IV catalytic cracking unit. ISA Transactions, 37, 215-226 (1998).

Fernandes, J. L., Pinheiro, C. I. C., Oliveira, N. M. C., Inverno, J. and Ribeiro, F. R., Model Development and Validation of an Industrial UOP Fluid Catalytic Cracking Unit with a High-Efficiency Regenerator. Ind. Eng. Chem. Res., 47, (3), 850-866 (2008).

Forbes, F., and Marlin, T. E., Design Cost: A Systematic Approach to Technology Selection for Model-Based Real-Time Optimization Systems, Comp. Chem. Engng., 20, 717-734 (1996).

Gouvêa, M. T. and Odloak, D., One-layer real time optimization in the FCC unit: procedure, advantages and disadvantages. Comp. Chem. Engng., 22, S191-S198 (1998).

Jacob S. M., Gross, B., Voltz, S. E. and Weekman, V. M., A Lumping and Reaction Scheme for Catalytic Cracking. AIChE, J., 22, (4), 701-713 (1976).

Kadam, J. V., Schlegel, M., Marquardt, W., Tousain, R. L., van Hessem, D. H., van den Berg, J. and

Bosgra, O. H., A two-level strategy of integrated optimization and control of industrial processes: a case study. In: European Symposium on Computer Aided Process Engineering, 12, 511-516, Elsevier (2002).

Kadam, J., Marquardt, W., Schlegel, M., Backx, T., Bosgra, O. H., Brouwer, P. -J., Dünnebier, G., van Hessem, D., Tiagounov, A. and de Wolf, S., Towards integrated dynamic real-time optimization and control of industrial processes. FOCAPO 2003 (Fourth International Conference on Foundations of Computer-Aided Process Operations) Coral Springs, Florida, 593-596 (2003).

Kadam, J. V., Schlegel, M., Srinivasan, B., Bonvin, D. and Marquardt, W., Dynamic Optimization in the Presence of Uncertainty: From Off-Line Nominal Solution to Measurement-Based Implementation. Journal of Process Control, 17, (5), 389-398 (2007).

Lang, Y-D., Cervantes, A. M. and Biegler, L. T., Dynamic Optimization of a Batch Cooling Crystallization Process. Ind. Eng. Chem. Res. 38, 1469-1477 (1999).

Lang, Y-D. and Biegler., L. T., A Software Environment for Simultaneous Dynamic Optimization. Comp. Chem. Engng., 31, (8), 931-942 (2007).

Logsdon, J. S. and Biegler, L. T., Accurate Solution of Differential-Algebraic Optimization Problems. Ind. Eng. Chem. Res., 28, 1628-1639 (1989).

Miletic, I. P. and Marlin, T. E., Results analysis for real-time optimization (RTO): Deciding when to change the plant operation. Comp. Chem. Engng., 20, S1077-S1082 (1996).

Miletic, I. P. and Marlin, T. E., On-line Statistical Results Analysis in Real-Time Operations Optimization. Ind. Eng. Chem. Res., 37, 3670-3684 (1998).

Odloak, D., Moro, L. F. L. and Spandri, R., Constrained Multivariable Control Of Fluid Catalytic Cracking Converters, A Practical Application. In: AIChE Spring Meeting, Houston. II., 84-90 (1995).

Odloak, D., Zanin, A. C. and Gouvêa, M. T., Integrating real-time optimization into the model predictive controller of FCC. Control Engineering Practice, London, 10, (8) 819-831 (2002).

Odloak, D., Robust Integration of RTO and MPC. In: 10th International Symposium on Process Systems Engineering – PSE2009, 119-126, Elsevier B.V. (2009).

Santos, M. G., Modelo Dinâmico para o Controle do Conversor de uma Unidade de FCC UOP STACKED. M.Sc. Thesis, Federal University of Rio Grande do Sul, UFRGS, Brazil (2000).

Secchi, A. R., Santos, M. G., Neumann, G. A. and Trierweiler, J. O., A Dynamic Model for a FCC UOP Stacked Converter Unit. Comp. Chem. Engng., 25, 851-858 (2001).

Srinivasan, B., Bonvin, D., Visser, E. and Palanki, S., Dynamic Optimization of Batch Processes: II. Role of Measurements in Handling Uncertainty Comput. Chem. Engng., 27, 27-44 (2003).

Srinivasan, B., Bonvin, D., Real-Time Optimization of Batch Processes by Tracking the Necessary Conditions of Optimality. Ind. Eng. Chem. Res., 46, 492-504 (2007).

Tanartkit, P. and Biegler, L. T., Stable Decomposition for Dynamic Optimization. Ind. Eng. Chem. Res., 34, 1253-1266 (1995).

Tanartkit, P. and Biegler, L.T., A Nested, Simultaneous Approach for Dynamic Optimization Problems – II: The Outer Problem. Comp. Chem. Engng., 21, 1365-1388 (1997).

Flores-Tlacuahuac, A., Saldívar-Guerra, E., Ramírez-Manzanarez, G., Grade Transition Dynamic Simulation of HIPS Polymerization Reactors. Comp. Chem. Engng., 30, 357-375 (2005).

Waanders, B. v-B., Bartlett, R., Long, K., Boggs, P. and Salinger, A., Large-Scale Non-Linear Programming for PDE Constrained Optimization. SAND2002-3198, Sandia National Laboratories (2002).

Wächter, A., An Interior Point Algorithm for Large-Scale Nonlinear Optimization with Applications in Process Engineering. PhD Thesis. Carnegie Mellon University, PA, United States (2002).

Zanin, A. C., Gouvêa, M. T. and Odloak, D., Industrial implementation of a real-time optimization strategy for maximizing production of LPG in a FCC unit. Comp. Chem. Engng., 24, 525-531 (2000a).

Zanin, A. C., Gouvêa, M. T. and Odloak, D., Comparing different real-time optimization strategies for the FCC catalytic converter. In: ADCHEM 2000 International Symposium on Advanced Control of Chemical Processes, Pisa (2000b).

Zanin, A. C., de Gouvea, M. T., Odloak, D., Integrating real-time optimization into the model predictive controller of the FCC system, Control Engng Practice, 10, (8), 819-831 (2002).

Zavala, V. M., Computational Strategies for the Optimal Operation of Large-Scale Chemical Processes, PhD Thesis, Carnegie Mellon University, PA, United States, pp. 65-70 (2008).

Zavala, V. M., Laird, C. D. and Biegler, L. T., Fast Implementations and Rigorous Models: Can Both be Accommodated in NMPC? International Journal of Robust and Nonlinear Control, 18, (8), 800-815 (2008).