NEW "CAPE" SOLUTIONS FOR OLEFINS PLANTS. DETAILED DYNAMIC SIMULATION AND DYNAMIC REAL-TIME OPTIMIZATION

Flavio Manenti[1*], Zohreh Ravaghi Ardebili[1], Nadson M. N. Lima[2], Lamia Zuniga Linan[2], Mattia Vallerio[3], Luca E. Viganò[4], Silvia Cieri[5], Marco Restelli[5], Tommaso Valcamonica[6], Marina Lopez Melgar[7], Giulia Piccioni[8], Matteo Cicciotti[1], Matteo D'Isanto[1], Paolo S. Carinci[1], Marco Gabba[1], Riccardo Borgomaneri[1], Nino Giannola[1], Alessandro Pulieri[1]

[1] Politecnico di Milano, CMIC dept. "Giulio Natta", Piazza Leonardo da Vinci 32, 20133 Milano, Italy
[2] University of Campinas, Department of Chemical Processes, Barão Geraldo, 13083-970, San Paolo, Brazil
[3] K.U. Leuven, BioTeC & OPTEC, Chemical Engineering Dept., W. de Croylaan 46, B-3001 Leuven, Belgium
[4] Saipem S.p.A., Chemical Process Technologies, Via Alcide de Gasperi 16, I-20097 San Donato Milanese, Italy
[5] Novartis Vaccines & Diagnostics, via Fiorentina 1, 53100 Siena, Italy
[6] Foster Wheeler Italiana S.r.l., Via S. Caboto 1, 20094 Corsico (MI), Italy
[7] University of Oviedo, Department of Chemical Engineering and Enviromental Technology, Avenida Julian Claveria 8, 33006 Oviedo, Spain
[8] International Thermal Technology S.p.A., Via Vasto 1, 20121 Milano, Italy
flavio.manenti@polimi.it

This paper deals with certain novel and appealing computer-aided process engineering (CAPE) solutions to improve flexibility, controllability, and operability of olefins plants. It shows the use of detailed kinetic schemes, developed and validated by Professor Sauro Pierucci and his colleagues at the Chemical Engineering group at Politecnico di Milano, to produce new effective tools for reliable and accurate dynamic simulation and dynamic real-time optimization methodologies. Preliminary results and tangible benefits are explained for a steam cracking furnace.

1. INTRODUCTION

Process dynamic simulation for the operator training and dynamic real-time optimization are the challenges of researchers in computer-aided process engineering (CAPE) community (Kadam et al., 2002; Lu, 2003; Tosukhowong et al., 2004; Lang and Biegler, 2007; Manenti and Rovaglio, 2008; Dones et al., 2010). Although, these issues are still perceived as an academic concept rather than industrial one, it seems it would has no wide applications the chemical plant they seems to be far from a massive use for online applications by the field. This is fundamentally due to the need to find simultaneously efficient and robust solutions so as to obtain accurate and effective results/previsions while ensuring their online feasibility for large-scale systems typical of process industry. This is the key-point: even though complex models able to characterize at best certain phenomena are available, we can use them in a few applications, since these are computationally too expensive to be used for online purposes. This is especially true in control and optimization disciplines of unit operations and production processes. Thus, by long time, since the advent of the digital era, we are forced to search for a good compromise between the level of detail of our models and the reasonable computational effort required for online (i.e. control or optimization) problems. In other words, The chemical plant continuously needs to use the reduced models to have effective and prompt responses. It unavoidably means that we accept less accurate but prompt solutions to manage industrial process and, therefore, that we accept myopic (suboptimal) set of actions and decisions in operating a plant.
Nowadays, we are undergoing a silent revolution in hardware and software systems and we can exploit two powerful tools to tackle the aforementioned issues: the object-oriented philosophy and the parallel computing.

The former deals with the software and specifically with the possibility to have more effective programming languages (Buzzi-Ferraris and Manenti, 2010a, 2010b); the latter deals with the spread of shared and distributed memory machines for numerical computing (Buzzi-Ferraris, 2010; Buzzi-Ferraris and Manenti, 2010c). Looking forward these tools, what was not reasonably possible yesterday, could be implemented today. This paper investigates the industrial feasibility of some appealing online solutions such as the dynamic simulation and the dynamic real-time optimization of chemical plants. A steam cracking furnace is selected as case study.

2. STEAM CRACKING FURNACE

Several methodologies can be adopted to crack heavy hydrocarbons to obtain light-ends. For the sake of conciseness we mention the fluid catalytic cracking, thermal cracking, and hydrocracking. The validation case it was selected focusing on the steam cracking, which produces ethylene and, in general, olefins from a feed of saturated hydrocarbons diluted with steam and then heated in a furnace (see the qualitative scheme of Figure 1).

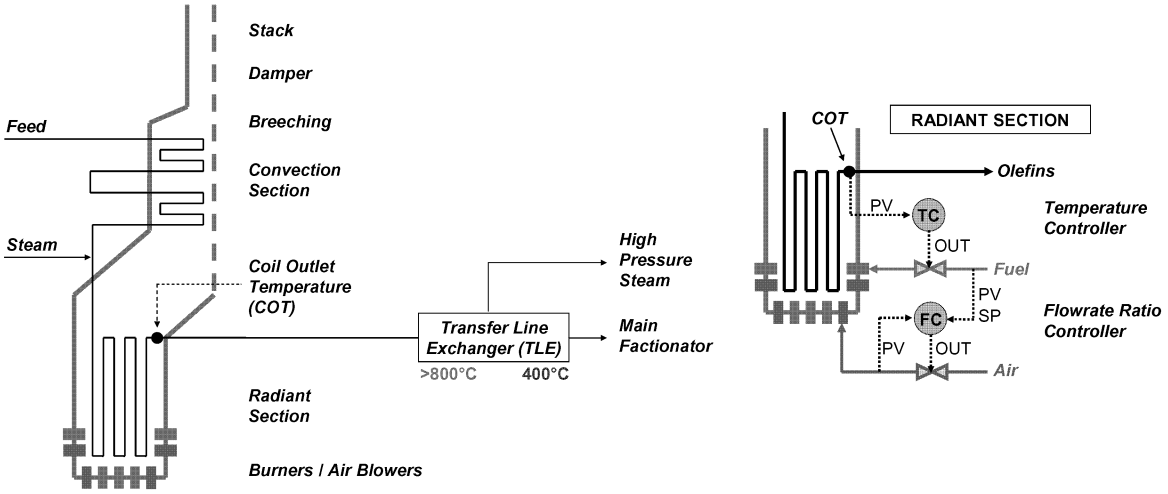

Figure 1. Half plan slice of a thermal cracking furnace (left-hand side); radiant section and related control scheme considered for the dynamic real-time optimization: PV stays for Process Variable, OUT stays for controller OUTput; and SP stays for SetPoint (right-hand side).

Before entering the radiant region, the feed flowrate is preheated in a series of heat exchangers placed in the convection region. In the thermal furnace, the temperature is considerably high (>800°C) and the residence time is in the order of some milliseconds (Dente et al., 1992). Here, one of the most important parameters to control and monitor the process performances is the coil outlet temperature (COT), which is measured before exiting the thermal furnace and is strictly related to the wall temperature. Therefore, the hot gas is quickly quenched in the transfer line exchanger (TLE) in order to stop the reaction and to produce high-pressure steam (about 100bar) as well. Assuming a fixed residence time, the outlet flowrate composition depends on the feed composition, the hydrocarbon to steam ratio, and the COT. The outlet flowrate is sent to the main fractionator and to the separation section (Pierucci et al., 1994; Pierucci et al., 1996). The main goal of this paper is to check the industrial feasibility of the dynamic simulation and dynamic optimization; it can be done by accounting for the radiant section only and its main control loops. In addition, efficiency degradation of the coil is not considered and other important parameters are intentionally neglected in this work. Nonetheless, it is worth remarking that a steam cracking furnace can usually run for a few months only at a time between de-coking operations. The selected control system related to the radiant section is reported in Figure 1. It consists of a direct-action temperature controller where the wall temperature of the radiant section, and hence the COT, is the controlled

variable and the fuel fed to the burners is the manipulated variable. A higher fuel flowrate corresponds to a higher COT value. A ratio controller manages the air flowrate insufflated into the radiant section, in order to maintain the desired stoichiometric ratio. The optimal setpoint is assigned by either the user or by the dynamic real-time optimizer, if any. The higher the fuel flowrate, the higher the air flowrate.

3. DYNAMIC SIMULATION

The dynamic simulation of chemical processes is the essential basis for many applications such as operator training simulators, nonlinear model predictive controls, and dynamic real-time optimizations to quote a few. The importance of dynamic simulation is testified by the recent spreading of several commercial packages to make easier the study of process dynamics and transients (Manenti, 2011). If, on one hand, these packages have large databases for chemical and physical properties, thermodynamic relations, and chemical species, on the other hand, their numerical kernel is not enough performing to ensure their use for online applications as the predictive control or the dynamic optimization. Actually, to simulate the process dynamics, we generally need differential and differential algebraic solvers; in addition, if we look forward online applications based on dynamic models, we need very performing and evenly reliable solvers for integrating numerically such systems. On this subject, we cannot anyhow neglect that when we speak about process dynamic simulation, we are indirectly speaking about process control and that the integral portion of the process control loops spoils the Jacobian structure of our system, by making computationally expensive the overall dynamic simulation. Specific solvers and devices are needed in these cases (Manenti et al., 2009). To benefit from the existing databases of commercial packages without losing in performances, to develop a dynamic simulation for the steam cracking furnace we integrated: (I) the BzzMath library solvers (BzzOde, BzzDae, BzzOdeNonStiff, BzzDaeSparse…), developed by Professor Guido Buzzi-Ferraris; (II) the SPYRO® model for cracking furnaces (Pyrotec-Technip), consisting of 300+ chemical species and 7000+ kinetic reactions; and (III) the DynSim™, the powerful dynamic simulation suite by SimSci-Esscor's Invensys Operations Management. A mixed-language approach has been adopted to merge SPYRO® (in FORTRAN language) with BzzMath and DynSim™ (both developed in Visual C++). By doing so, we obtained a fully integrated and fully synchronized dynamic simulation of a steam cracking furnace, which is based on a very detailed model and solved by algorithms exploiting object-oriented programming and parallel computing. To validate the overall system we supposed that the market prices of ethylene and propylene change by requiring different severity values to have an optimal production. A dynamic simulation for the propylene/ethylene severity change (0.62 to 0.67) is reported in Figure 2. Olefins plant data are given elsewhere (Pierucci *et al.*, 1994; Pierucci *et al.*, 1996) for the sake of conciseness.

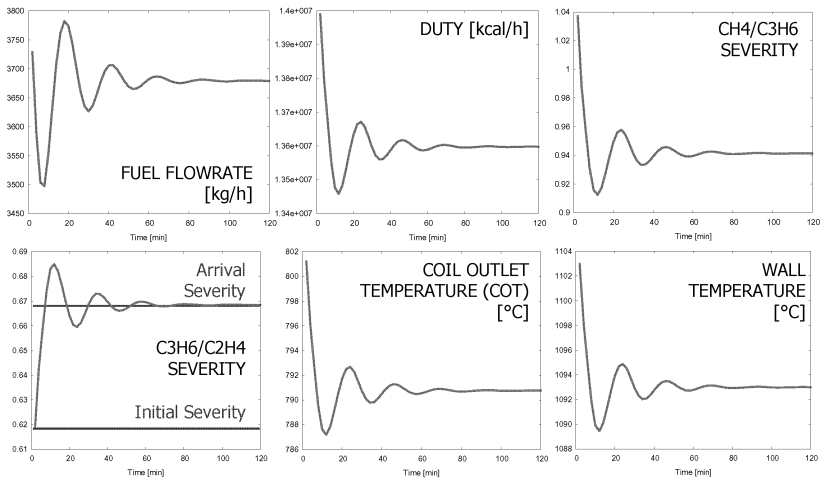

Figure 2. C_3H_6/C_2H_4 Severity Change from 0.62 to 0.67 imposed by market price dynamics

Figure 2 shows the fuel flowrate fed to the burners of the selected furnace, the corresponding duty supplied to the radiant section, the methane/propylene severity, the propylene/ethylene severity, the COT, and the wall temperature of the radiant section. The new propylene/ethylene severity imposed by the market price fluctuations is achieved after 65 min. A dynamic simulation of 2h takes 2s of CPU on a common QUADCORE machine.

4. DYNAMIC REAL-TIME OPTIMIZATION

Speaking about process transients and looking at the trends of Figure 2, a question is: could we optimize the path of each severity change? If so, could we reduce their duration, oscillations, and instabilities? Could we have relevant economical benefits from it? Let us start saying that the dynamic simulation has assumed more and more importance in these decades not only for control system validation and process safety analysis, which are its traditional uses, but also for **the ability we have to foresee the future behavior of the processes when detailed dynamic models are available**. This is the very foundation of the dynamic real-time optimization that makes it different from the traditional (steady-state, not dynamic) real-time optimization. The dynamic optimization is similar in its mathematical formulation and time-scale to the nonlinear model predictive control, another optimization level of the so-called process control hierarchy (Busch et al., 2007): they involve only continuous variables, whereas strategic levels such as scheduling and planning requires also discrete variables (Floudas, 1995); they are based on the moving horizon methodology (Rawlings, 2000); they are both a multidimensional, constrained, nonlinear programming (NLP) problems based on convolution models, often requiring specific optimizers and differential solvers (Buzzi-Ferraris and Manenti, 2010c). Differences between the dynamic optimization and the nonlinear model predictive control problems can be summarized in few sentences: the nonlinear model predictive control is traditionally a quadratic control problem, whereas the dynamic optimization accounts for market dynamics; degrees of freedom of the resulting NLP are the manipulated variables for the nonlinear model predictive control and the setpoints for the dynamic optimization; the objective function is usually a sum of least squares for the nonlinear model predictive control, whereas the dynamic optimization usually preserves this form in the anti-ringing terms only. In short, the nonlinear model predictive control is aimed at driving the plant from the current operating conditions to a new set of economically optimal conditions along an optimized set of setpoint trajectories; the new setpoint trajectories are defined by the dynamic optimization that accounts for market dynamics, demand uncertainty, price volatilities, cost fluctuations… By doing so, the plant operates close to its optimum also when it undergoes persistent disturbances, partial loads, grade change transitions, or process transients in general.

4.1 Solution strategies

Two solutions are available for the dynamic optimization and they differ on the discretization type adopted for the constraints within the optimization problem (Biegler and Hughes, 1982, 1985): sequential and simultaneous methods. In the *sequential methods*, the dynamic model is kept separate from the optimizer; the model simulation and the optimization are performed sequentially, and the convolution model is numerically integrated along the prediction horizon at each iteration of the optimizer. These approaches are also called the *partially parameterized methods*, since manipulated variables only are discretized, and the *feasible path methods*, since a feasible solution of the dynamic system is needed at each iteration. In the *simultaneous methods*, the dynamic model is fully discretized as per manipulated variables and it is directly integrated in the optimization problem. It is not a case that these approaches are sometimes called the *fully parameterized methods*. They are also named the *infeasible path methods*, since it is not necessary to have feasible solutions of the dynamic model (except for the last iteration) as the numerical integration and the optimization simultaneously converge. An important class of these methods is the so-called multiple shooting method (Tanartkit and Biegler, 1995; Leineweber et al., 2003). Both methods have advantages and disadvantages. The simultaneous one brings to a sparse structured system that could be integrated by very performing solvers (Manenti et al., 2009), but dimensions of the resulting nonlinear programming problem are unavoidably enlarged. On the other hand, the sequential approach preserves the size of the optimal problem and it is easier to implement, but it is usually more computationally

expensive than the simultaneous, one since more iterations are needed to continuously get a solution for the dynamic system. The multiple shooting approach belonging to the family of simultaneous methods is adopted in the present research activity (Diehl, 2001):

$$
\begin{aligned}
&\Phi = \min \int_0^T L\left(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t)\right)dt \\
&s.t.: \\
&\dot{\mathbf{x}}(t) = f\left(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t),p,t\right) \\
&0 = g\left(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t),p,t\right) \\
&\mathbf{x}(0) = \mathbf{x}_0 \\
&h\left(\mathbf{x}(t),\mathbf{z}(t),\mathbf{u}(t)\right) < 0
\end{aligned}
\quad \rightarrow \quad
\begin{aligned}
&\Phi\left(\mathbf{x}_0\right) = \min_{\substack{\mathbf{q}_0,\ldots,\mathbf{q}_{N-1} \\ \mathbf{s}_0,\ldots,\mathbf{s}_N}} \sum_{i=0}^{N-1} \Phi_i\left(\mathbf{s}_i,\mathbf{q}_i\right) \\
&s.t.: \\
&\mathbf{s}_{i+1}^x - \mathbf{x}_i\left(\tau_{i+1};\mathbf{s}_i,\mathbf{q}_i\right) = 0 \qquad i = 0,1,\ldots N-1 \\
&g\left(\mathbf{s}_i^x,\mathbf{s}_i^z,\mathbf{q}_i\right) = 0 \qquad i = 0,1,\ldots N \\
&\mathbf{s}_0 - \mathbf{x}_0 = 0 \\
&h\left(\mathbf{s}_i^x,\mathbf{s}_i^z,\mathbf{q}_i\right) \geq 0 \qquad i = 0,1,\ldots N
\end{aligned}
\tag{1}
$$

where $\mathbf{q}_i$ and $\mathbf{s}_i$ are the sets of discretized manipulated and state variables ($\mathbf{u},\mathbf{x}$), respectively, in the τ_i intervals of the time horizon T; the objective function Φ is subject to differential and algebraic equations (f,g), initial conditions $\mathbf{x}_0$, and inequality constraints h. Using a set of performing optimizers (Buzzi-Ferraris and Manenti, 2010c; Manenti et al., 2010), the dynamic simulation of the previous paragraph, obtained combining SPYRO®, BzzMath, and DynSim™, can be iteratively called in order to evaluate the best setpoint trajectory to drive the steam cracking furnace from a set of operating conditions to the new set imposed by the severity change. To emphasize the benefits of dynamic optimization, a relevant severity change is imposed to the steam cracking furnace. The convergence path of the industrial best practice is compared to the dynamic optimization path (Figure 3). Trends for the fuel flowrate fed to the burners are given in Figure 4.

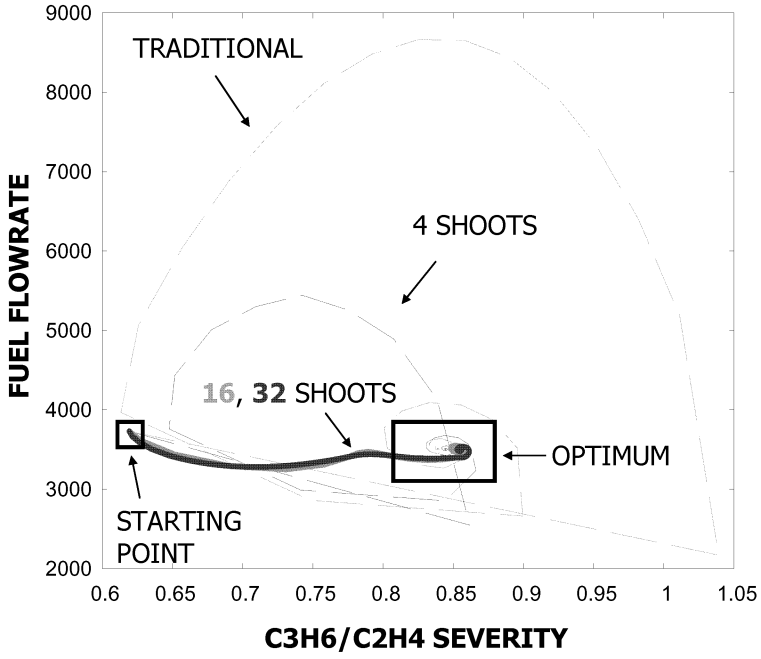

Figure 3. C_3H_6/C_2H_4 severity change converging path (fuel flowrate in kg/h). Real-time optimization (traditional approach) versus dynamic real-time optimization.

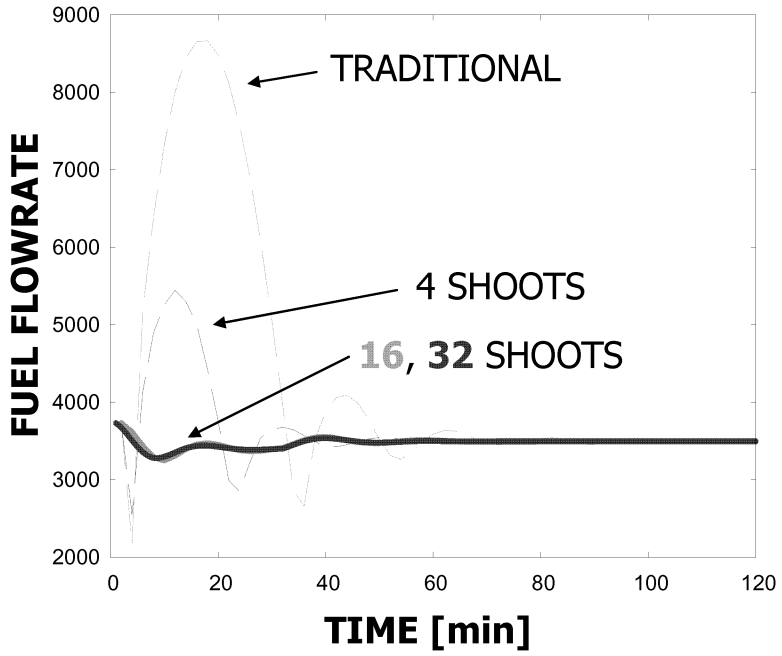

Figure 4. C_3H_6/C_2H_4 severity change: fuel flowrate [kg/h] fed to burners. Real-time optimization (traditional approach) versus dynamic real-time optimization

It is worth saying that an increase in the number of shoots corresponds to an increase in the computational effort. Nevertheless, using a few of shoots (e.g. 16 or 32), the computational effort is practically the same of the steady-state real-time optimization on a common QUADCORE machine, whereas the benefits in plant stability, flexibility, and controllability are clear: no relevant changes in the fuel flowrate during the operational severity change; no oscillations of the steam cracking furnace; faster achievement of the new (optimal) operating conditions.

5. CONCLUSIONS

This research activity demonstrated the online feasibility of certain new CAPE solutions for olefins plants. The detailed dynamic simulation of a steam cracking furnace has been obtained by combining SPYRO®, BzzMath library, and DynSim™. This dynamic simulation has been used as convolution model to implement the dynamic real-time optimization. The preliminary results showed the economical appeal of these novel CAPE solutions, not only in terms of production yield, but also for the improved plant flexibility, stability, and controllability.
Looking forward the more and more stringent regulations for environmental safeguard and the more frequent production changes imposed by market price volatilities of oil and chemical commodities, the dynamic simulation and the dynamic optimization seems to be two promising methodologies for process control and optimization purposes in the next future on the industrial scale.

6. REFERENCES

Biegler, L.T., & Hughes, R.R., 1982, Infeasible Path Optimization with Sequential Modular Simulators. AIChE J. 28(6), 994-1002.

Biegler, L.T., & Hughes, R.R., 1985, Feasible Path Optimization with Sequential Modular Simulators. Computers & Chemical Engineering 9, 379-394.

Busch, J., Oldenburg, J., Santos, M., Cruse, A., & Marquardt, W., 2007, Dynamic Predictive Scheduling of Operational Strategies for Continuous Processes Using Mixed-logic Dynamic Optimization. Computers & Chemical Engineering 31, 574-587.

Buzzi-Ferraris, G., & Manenti, F., 2010a, Fundamentals and Linear Algebra for the Chemical Engineer: Solving Numerical Problems. Wiley-VCH, Weinheim, Germany.

Buzzi-Ferraris, G., & Manenti, F., 2010b, Interpolation and Regression Models for the Chemical Engineer: Solving Numerical Problems. Wiley-VCH, Weinheim, Germany.

Buzzi-Ferraris, G., 2010, New trends in building numerical programs. Computers and Chemical Engineering doi:10.1016/j.compchemeng.2010.07.004.

Buzzi-Ferraris, G., & Manenti, F., 2010c, A Combination of Parallel Computing and Object-Oriented Programming to Improve Optimizer Robustness and Efficiency. Computer Aided Chemical Engineering 28, 337-342.

Dente, M., Pierucci, S., Ranzi, E., & Bussani, G., 1992, New Improvements in Modeling Kinetic Schemes for Hydrocarbon Pyrolysis Reactors. Chemical Engineering Science 47(9-11), 2629-2634.

Diehl, M., 2001, Real-Time Optimization for Large Scale Nonlinear Processes. PhD Thesis, IWR, University of Heidelberg, Heidelberg.

Dones, I., Manenti, F., Preisig, H.A., & Buzzi-Ferraris, G., 2010, Nonlinear Model Predictive Control: a Self-Adaptive Approach. Industrial & Engineering Chemistry Research 49(10), 4782-4791.

Floudas, C.A. (1995). Nonlinear and Mixed-Integer Optimization - Fundamentals and Applications. New York, NY, USA.

Kadam, J.V., Schlegel, M., Marquardt, W., Tousain, R.L., van Hessem, D.H., van der Berg, J., et al., 2002, A Two-level Strategy of Integrated Dynamic Optimization and Control of Industrial Processes - a Case Study. ESCAPE-12, The Hague, The Netherlands, 511-516.

Lang, Y.D., & Biegler, L.T., 2007, A Software Environment for Simultaneous Dynamic Optimization. Computers & Chemical Engineering 31, 931-942.

Leineweber, D.B., Bauer, I., Bock, H.G., & Schloder, J.P., 2003, An Efficient Multiple Shooting Based Reduced SQP Strategy for Large-scale Dynamic Process Optimization. Part 1: Theoretical Aspects. Computers & Chemical Engineering 27(2), 157-166.

Lu, J.Z., 2003, Challenging Control Problems and Emerging Technologies in Enterprise Optimization. Control Engineering Practice 11(8), 847-858.

Manenti, F., & Rovaglio, M., 2008, Integrated multilevel optimization in large-scale poly(ethylene terephthalate) plants. Industrial & Engineering Chemistry Research 47(1), 92-104.

Manenti, F., 2011, Natural Gas Operations: Considerations on Process Transients, Design, and Control. ISA Transactions, accepted paper.

Manenti, F., Dones, I., Buzzi-Ferraris, G., & Preisig, H.A., 2009, Efficient Numerical Solver for Partially Structured Differential and Algebraic Equation Systems. Industrial & Engineering Chemistry Research 48(22), 9979-9984.

Manenti, F., Buzzi-Ferraris, G., Pierucci, S., Rovaglio, M., & Gulati, H., 2010, Process Dynamic Simulation Using ROMeo. Computer Aided Chemical Engineering accepted paper.

Pierucci, S., Faravelli, T., & Brandani, P., 1994, A Project for On-line Reconciliation and Optimization of an Olefin Plant. Computers & Chemical Engineering 18, s241.

Pierucci, S., Brandani, P., Ranzi, E., & Sogaro, A., 1996, An industrial application of an on-line data reconciliation and optimization problem. Computers & Chemical Engineering 20, S1539-S1544.

Rawlings, J.B., 2000, Tutorial Overview of Model Predictive Control. IEEE Control Systems Magazine 20(3), 38-52.

Tanartkit, P., & Biegler, L.T., 1995, Stable Decomposition for Dynamic Optimization. Industrial & Engineering Chemistry Research 34(4), 1253-1266.

Tosukhowong, T., Lee, J.M., Lee, J.H., & Lu, J., 2004, An Introduction to a Dynamic Plant-wide Optimization Strategy for an Integrated Plant. Computers & Chemical Engineering 29(1), 199-208.