A Framework for On-line Full Optimising Control of Chemical Processes

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Abstract
An increasing demand for improved productivity and better quality control has shifted the interest of the research community to nonlinear model-based control, which has a better chance to meet these requirements due to the intrinsic nonlinear nature of chemical and physical processes. Recent progress in modelling, simulation and optimisation environments (MSOEs) and open software architectures (OSAs) have created the conditions to conceive novel paradigms for advanced process control (APC) of large-scale complex process systems. However, large-scale mechanistic models have scarcely been used in control algorithms and, therefore, issues arising from embedding these process models in APC applications have not been addressed satisfactorily. In this manuscript we propose a novel framework for advanced nonlinear model-based control of process systems which aspires to bring the latest advances in model-based technology closer to the Process Industries.

1. Introduction
Nowadays, not only state-of-the-art MSOEs support efficiently most stages of the modelling process, but also allow the creation of large-scale mechanistic models and solution of advanced model-based activities that were impossible to engage in one decade ago (Pantelides, 2001). Additionally, as rigorous process models conforming to the CAPE-OPEN (CO) standards proliferate in the public domain of the PSE and CAPE communities, the time and effort to develop large-scale mechanistic models is reduced considerably. Even though these mathematical models could be used as precursors of advanced model-based control algorithms, the research community has failed to provide a framework to use rigorous mechanistic models in APC applications. Undoubtedly, MSOEs and OSAs have driven major changes in model-based technology and will continue to promote further transformations. However, how to benefit from MSOEs and OSAs to conceive new visions and establish novel paradigms in the area of APC is still an unresolved question. In this work, we present to the research community and industry the most important aspects of the framework for full optimising control of process systems (FOCoPS) proposed by Rolandi (2004).

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2. Framework Definition

2.1. Control algorithm and general philosophy

The framework is centred on hierarchical control architecture where multivariable constrained control and process optimisation (which were traditionally segregated into distinct layers (e.g. Qin and Badgwell, 1996)) are combined into a single hierarchical level. A rigorous mechanistic dynamic model of the process is used for this purpose.

The core of the proposed control algorithm is based on the on-line iterative solution at time \( t = t_0 - \Delta \) of a finite horizon open-loop optimal control problem (FHP) of the form:

\[
\min_{\tilde{u}(t) \in \tilde{U}(t_0, t_0 + \Delta)} \phi(t_0 + \Delta)
\]

\[F(\tilde{x}(t), x(t), y(t), u(t)) = 0, \quad t \in \left[ t_0, t_0 + \Delta \right]
\]

\[I(\tilde{x}(t_0), x(t_0), y(t_0), u(t_0)) = 0
\]

\[\tilde{u}(t) = \tilde{u}(t_0 + C \cdot \Delta), \quad t \in \left[ t_0 + C \cdot \Delta, t_0 + \Delta \right]
\]

\[\tilde{u}(t) \in U, \quad t \in \left[ t_0, t_0 + \Delta \right]
\]

\[y(t) \in Y, \quad t \in \left[ t_0, t_0 + \Delta \right]
\]

\[x(t) \in X, \quad t \in \left[ t_0, t_0 + \Delta \right]
\]

The nomenclature conventions adopted in the equations above are straightforward. The symbols \( P \), \( C \) and \( \Delta \) denote the prediction horizon, the control horizon and the control window, respectively. Additionally, \( \tilde{u}(t) \) indicates the subset of controlled input variables. In the proposed architecture, these decision variables correspond to the set-points of the regulatory (PID) control layer. The FHP is solved via a control vector parameterisation approach, or sequential solution method, with piecewise-constant controls \( \tilde{u}^A \in U \). Details on feedback mechanisms and other features of the control algorithm can be found in Rolandi (2004).

In the proposed framework for FOCoPS, we suggest to differentiate the objective function (i.e. Eq. (1), a primary and direct performance measure) from the series of process constraints on state and output variables that define the admissible set of trajectories (i.e. Eqs. (6) and (7), secondary and indirect measures of performance). In effect, objective functions such as productivity or overall profitability are more intuitive and natural performance measures for the purpose of simultaneous process optimisation and control than the multivariable objective function typically encountered in linear model-predictive control (LMPC) applications. However, translating the constraints arising from a control problem into equivalent terminal and path constraints of the corresponding NLP problem formulation and simultaneously guaranteeing the existence of a non-empty feasible region is a non-trivial problem. We will address this issue in subsequent sections of this paper.

The reader may feel persuaded to think that the rupture with the multivariable constraint dynamic control (or quadratic cost) objective function and consequent reduction of the
number of algorithmic parameters (i.e. elimination of weighting matrices intrinsic to any multivariable objective function) is a drawback of the proposed framework. On the contrary, in the author’s opinion, it represents a paradigm shift that holds the potential for significant boost of the process systems performance due to a more realistic treatment of process constraints given by the specification of the control problem. Effectively, Prett and Garcia (1988) recognised that performance requirements cannot be appropriately reflected by the combination of multiple objectives into a single objective function. For instance, not only should control requirements be translated into appropriate relative weights, but care should also be exercised to avoid scaling problems and ill-conditioned solutions (Qin and Badgwell, 1996). Ultimately, the weights are used as tuning parameters of the control algorithm balancing the relative enforcement of admissible input and output trajectories.

On the contrary, in the proposed framework, the performance of the controller is intimately associated with the structure of the control problem, that is, the characteristics of the objective function, and number and nature of the control variables and constraints. Since these reflect true specifications of the required process operation, better control performance can be expected from the proposed framework.

2.2. On-line formulation of the control problem

The framework for FOCoPS has been centred on the initiative of translating a process control problem into an equivalent NLP formulation, and then converting this problem into a high-level declarative definition consistent with the native language of state-of-the-art MSOEs. Even though this is an important conceptual breakthrough, several complications arise since the control problem is likely to be stated by the user (e.g. an operator) in a very straightforward way, with little resemblance with the conventions of modern modelling languages.

In order to fulfil this vision, the FOC/APC application currently supports the following mechanisms: a) the user has the ability to communicate with the application kernel by posting a series of elementary events describing the structure of the control problem at discrete points in time; b) concurrently, the application kernel has the capacity to translate this series of future events posted by the user into an equivalent NLP problem. The elementary event data model (EVNm) has been suggested as an abstraction of all relevant information that should be contained in an event to make it useful for the purpose described above (Rolandi, 2004). Additionally, a dynamic optimisation object data model (DOOdm) was created to represent the high-level declaration of the NLP/FHP within the FOC/APC application. Since the conventions of gPROMS’ high-level declarative language were used to describe the mathematical form of the NLP problem, the generation of the gPROMS language input file describing a dynamic optimisation problem given by the DOOdm was straightforward.

The control problem definition and solution supervisor (CPDaSS) is the software component of the FOC/APC application in charge of manipulating instances of the EVNm and transforming them into a DOOdm. The algorithmic nature of this component is fairly involved and research is still being conducted in this area. In spite of this, a general discussion of the issues involved during such translation and associated software implementation aspects can be found in Rolandi (2004).
2.3. Advanced features of the framework

In industrial processing plants, input process variables may be “lost” due to hardware or software signal failure or unavailable due to direct intervention from the operator or the supervisory control system. Concurrently, constraints on output process variables may be modified due to alterations on process operation specifications. On the other hand, solution ill-conditioning may result from poor control problem definition or abnormal process performance, and an adequate modification of configuration (input and/or output variables, Eqs. (5) and/or (6)) could be used to recover from this situation. All of these circumstances cause the structure of the control problem to change dynamically.

In the proposed framework for FOCoPS, changing the structure of the control problem is possible via the introduction of a series of mechanisms which allow a flexible definition of the associated on-line NLP/FHP. These mechanisms respond to the type of elementary event. At the moment ten different types are supported. **PH_Change**, **CH_Change** and **CW_Change** keywords trigger changes in the prediction horizon, control horizon and control window respectively, thus affecting the nature of the multi-stage dynamic optimisation problem. **PC_Create** and **PC_Delete** are used to modify the structure of piecewise-constant decision variables of the NLP problem. For instance, **PC_Create** adds an additional control variable and/or modifies the magnitude of upper and lower bounds and initial guesses of an already-existent control variable. In addition, **PC_Delete** removes a piecewise-constant control variable from the list of decision variables. **FR_Create** and **FR_Delete** are used for similar purposes for the case of process constraints, while **FR_Create_FixedEndPoint** and **FR_Delete_FixedEndPoint** are special cases of the latter and are needed when the occurrence time of the elementary event is always coincident with the end of the prediction horizon. Finally, **OV_Change** allows the user to change the process variable reflecting the objective function.

At the moment, the user is the driving force in the definition of the control structure because the elementary events can only be posted by a restricted set of mechanisms. It is important to highlight, though, that such elementary events could be initiated by internal and/or other external agents to the FOC/APC application.

The opportunity to modify the NLP formulation on-line by posting elementary events gives good flexibility and generality to the framework. In spite of this, it also gives rise to several non-trivial issues such as guarantying the validity and feasibility of the newly created NLP problem. Effectively, problem infeasibility or ill-conditioning may occur as a result of abnormal process operation and/or an intrinsically badly-posed control problem. In the FOC/APC application, constraint ranking and elimination was exploited as a mechanism for recuperation form infeasible solutions. In other words, when the solution of the NLP problem becomes infeasible, constraints below a priority level are eliminated from the formulation and the calculation is repeated. The NLP is considered infeasible for the purposes of implementation only when constraints above a certain priority level cannot be enforced. In addition, constraint identification and relaxation has been proposed as a complementary approach to infeasibility recuperation (Rolandi, 2004), although the lack of standard methods for communication with numerical solvers hails the implementation of this idea for the moment. Infeasibility recuperation is handled by the control problem definition and solution supervisor (CPDaSS), since the
function of this component is to respond to control problem formulations that change dynamically according to endogenous or exogenous reasons.

3. Implementation

State-of-the-art MSOEs such as gPROMS provide standard mechanisms to interact with the modelling and solution engine at a lower level than the conventional model development and activity execution environment. This is accomplished via the gPROMS Server (gSERVER), which allows any application to construct process models in gPROMS’ native language, perform all supported model-based activities, and have full access to the mathematical description of the corresponding models and activities as specified by the GCO standard. The FOC/APC application has been implemented in C++ object-oriented programming language, although some components will support XML soon.

4. Results and Discussion

In this manuscript, the framework is presented and exemplified through a case study. The process under consideration is a continuous cooking digester and auxiliary units. A large-scale model consisting of approximately 14000 algebraic and 1000 ordinary differential equations (DAEs) and 100 statuses within the state transition network (STNs) is the process model used by the FOC/APC algorithm. This model has been implemented in gPROMS modelling language. The communication between the virtual (simulated) process system (VPS) and the FOC/APC application is accomplished via Honeywell Experion PKS™ by means of the network application programming interface (NAPI) protocol.

The viability and performance of the FOC/APC application is assessed by the following illustrative case-study. Let us assume that the results of an off-line study seeking to find the optimal transition management procedure for slowing down the production from 650.0 to 600.0 ad.ton/day is available to mill personnel. In this study, pulp yield was maximised while keeping the deviation of pulp selectivity from its target operating value below a given threshold for quality control. Typically, these transition planning case-studies would be obtained under the assumption that the process system was initially operating at steady-state. Let us assume, instead, that a production rate change from 600.0 to 650.0 ad.ton/day had taken place five hours before the new transition (following similar optimality criteria, though). By doing this, we would like to support the thesis that results from off-line process optimisation and transition planning studies are useful to indicate the direction for enhancement of the process operation but are not directly applicable as control recipes unless process performance is sacrificed.

The transition is accomplished by manipulating the set-point of three controllers: the chip meter speed (feed rate of wood chips), and the temperature of the lower and wash circulation heaters (indirect column heating). Path (interior-point) and terminal (end-point) constraints were imposed on the trajectories and final magnitude of blow-line kappa number and blow-line pulp production rate. Two additional (en-point) constraints were added for the deviation and violation of soft-control bounds of the kappa number. The prediction and control horizons were 7hr and 5hr, and the control window was 1hr.
Figures 1 and 2 compare the trajectories of key process variables for the transition based on process knowledge derived off-line (OFL) and that driven by the on-line FOC/APC control algorithm (ONL). It is clear that the FOC/APC application was able to manage the transition more efficiently than what operators could have done on the basis of previous process knowledge.

![Graphs showing trajectories](image)

**Figure 1: Kappa number trajectory.**  **Figure 2: Lower heater set-point trajectory.**

### 5. Conclusions

This work presented a novel framework (FOCoPS) for on-line optimising control of large-scale processes. The emphasis was centred on creating a paradigm which would support the definition of a control problem in a way consistent with the structure and formalisms of high-level declarative languages and the framework imposed by the CO standards. The innovative *elementary event data model* was presented as a means to change the structure of the control problem dynamically due to the interaction of the APC application with the operators and the process system.

A large-scale mechanistic process model of an industrial continuous pulping area was used to illustrate the framework. In this work, only key issues of the novel framework have been addressed, and no attempt has been made to compare the proposed algorithm with other standard model-based control technologies such as LMPC. However, the framework is expected to bring improved process profitability and quality control because optimisation and control occur simultaneously in the proposed architecture for FOCoPS and the FOC/APC application is centred on mechanistic process models.

Overall, this paper has provided a framework for advanced process control (APC) compatible with the paradigm for open software architectures (OSA) given by the Global CAPE-OPEN (GCO) project. Naturally, the PSE, CAPE and APC community will greatly benefit from further research in the path delineated by this manuscript.

### 6. References

- Pantelides, C.C., 2001, New challenges and opportunities for process modelling, ESCAPE-11, Kolding, Denmark.