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Scalable integrated solution for real time estimation, control and optimization of the quality of fuels manufactured in refineries: an industrial story

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Abstract: This article reports the developments of the technology used at TOTAL for estimating, controlling and optimizing the quality of fuels produced in refineries. Some key difficulties and practical problems are discussed along with a schematic description of the developed solutions and on-going research efforts.

Keywords: Process Control; Production planning and control; Systems interoperability; Fuel blending; Optimization

1. INTRODUCTION

Integrated real-time automation and optimization related to the process of blending petroleum bases in refineries has developed remarkably over the past years, both technically and scientifically. Generally, the problem of fuel blending is of great industrial importance and has received considerable attention (see e.g. Perkins (2000); Bay et al. (1969); Feld et al. (1968); Le Febre and Lane (1995); Singh et al. (2000) and references therein).

This article presents some of the results obtained at TOTAL, roughly over the last two decades. This paper is presented from an industrial viewpoint, and aims at presenting the challenges, the technologies at stake and some solutions that have emerged to tackle these issues. Numerous details not covered here can be found in Bernier et al. (2006); Chèbre et al. (2010a, 2011); Chèbre (2006); Chèbre and Pitollat (2008).

The integration leading to the creation of the technology currently used was initially a technical matter, with the inclusion of optimization solutions in the latest generation of product movement software suites from Distributed Control Systems (DCS) suppliers, using standard interoperable communication interfaces for reading and writing.

Along with these technical advances in integration and automation (which mainly aimed at improved scalability and maintainability), estimation and control algorithms have been developed to respond to production-related changes. In particular, the production of sulfur-free fuels and biofuels have been strong driving forces behind these developments.

2. CONSTRUCTING INTEROPERABILITY ON THE TECHNOLOGICAL PLATFORM

Standardized communication interfaces for exchanging useful data with the various (and different) DCS used in factories have been built for blending units. This is a major prerequisite for secure interoperability which, in turn, allows easy and agile deployment of software in refineries in an environment of latest-generation production automation based on a single shared-platform. XML and OPC communication protocols were used to establish read-write secure data exchange. This standard scheme has been applied to both the off-line blend recipe preparation tool and the on-line fuel blend control and optimization software.

To achieve such interoperability, an integration project was launched with a steering committee that included industrial management, consultants, and two teams of specialists from suppliers. Two pilot sites participated in the preliminary feasibility study and the specification and detailed design phase: Donges (France) with a Honeywell DCS and Leuna (Germany) with a Schneider Electric DCS.

The integrated solution is now operational in Port Arthur (USA) with the BMA (Blend Movement Automation) software suite by Honeywell and in Leuna with the BOSS (Blend Optimization and Supervisory System) suite, see P.J. Walton (2003). It has also been implemented at the Donges refinery in 2016.

Integration was done with standard interfaces for connection to outside environments (suppliers). TOTAL in-house tools were also integrated: ANAMEL (a tool for real-time closed-loop optimization of fuel manufacturing recipes Bernier et al. (2006); Chèbre et al. (2010b)) and OPTIS (a tool for off-line preparation of recipes for blending batches to be produced). For those tools, the evolution concerned not only the form, connecting interfaces-exchanges using XML files - but also the content, harmonizing optimization criteria and ensuring the convergence of computing kernels.

The aim of the coupling was to increase the reliability of the reference recipes used at the start of production, with two objectives: to avoid infeasible cases that might cause delays in launching blending batches and to accelerate convergence thanks to a more representative initial recipe. This ensures the earliest possible compliance with the specifications for the fuel that is produced, which is of great importance in the context of on-line certification of finished products.

3. DEVELOPMENT OF THE ESTIMATION-CONTROL-OPTIMIZATION PLATFORM

Simultaneously with the works described above, scientific developments on the control kernel of blending have made constant progress. The improvements mainly concern key features of the in-house ANAMEL software. In particular, the optimization kernel and the algorithm used to estimate in real-time the qualities of the bases being blended during fuels production have both been the subject of numerous research works.

In ANAMEL, a blending model is adaptively adjusted based on periodic measurements by *online analysers* of the final blend product (the commercial fuel). The initial values of the components quality estimates are laboratory analyses of each component, for each property. The main algorithm consists of two distinct, connected layers: an optimization problem and a feedback loop with an observer. The optimization problem accounts for various constraints and production cost minimization. The observer is used to (partially) estimate the components properties in a spirit of adaptive control methods. Interestingly, to provide convergence of the blend properties to a prescribed target, ANAMELs observer needs not to converge to the actual unknown values of the components properties. This might be the case though, but may not be so common in practice. Most of the time, the blend target is reached before accurate estimates of the components properties are obtained. This is not a concern, because blend properties are definitely the primary target. This behavior is analyzed using LaSalle's invariance principle for the underlying dynamical system (Chèbre et al. (2010b)).

There has been a series of projects related to the adaptation scheme of the model (including standardization of the governing adaptation law, scaling, and acceleration of convergence, integration of positivity constraints, percentage limits for distillation, rankings to be satisfied by the estimates). Associated guarantees of asymptotic convergence were theoretically established each time. In details, the adaptation laws of ANAMEL have been updated with additional terms in the right-hand-side of the observer differential equations, or, as an alternative, periodic reset of the observer state is performed at discrete times. The first solution guarantees that the ranking and bounds are satisfied asymptotically. Again, this fact is guaranteed by a careful geometric study of the LaSalle's invariance set eventually reached by the system, which was performed in Chèbre et al. (2011). The second solution considers an optimization problem to periodically compute corrections to the estimator state. Such optimization problems are proven to possess unique solutions by means of Farkas' lemma (using the formulation of Nering and Tucker (1993)).

Improvements were also made to the normalization strategy of the estimator in order to allow a directed redistribution of the prediction error. This work was carried out to address the need (which was particularly critical at Donges) for a really fine estimate of the absolute value of the quality of blending bases when they are not measured - for example in cases where the relevant value is outside the analyser range. The difficulty of this work was in fact to estimate not a relative value of the bases quality (generally sufficient for controlling the qualities in closed-loop) but their absolute value in a fashion also in open-loop.

The discretization scheme of the differential equation that adapts the model was reconsidered, and its stability for large and varying sampling steps was improved.

Then, it appeared to be necessary to take into account uncertainties of various types and to imagine new solutions to refine the estimates. One source of uncertainty is that the variability in the quality of oil bases sometimes results from the practice known as "inflow-outflow". The component tanks are subjected to movements by products entering and leaving simultaneously, with the entering flows coming from upstream treatment units and a flow leaving the blender located downstream collecting the flows leaving each of the tanks for a component to be used in the blend. The lack of product homogenization in the tanks and stratification resulting for the absence of agitators can lead to non representative sampling and thus laboratory measurements do not reflect to field reality. More generally, uncertainties of various kinds are taken into account here: repeatability of measurements, direct run-down common practice for blend component tanks, product tank heels quality estimation without lines volume flushing being taken into account, approximation of the blending law modeling conversion for the linearization step, pre-blended products upstream to the fuel blender.

Uncertainties on the measurements by the on-line analysers can also occur. Approximations of regressive blending models used in linear index transformations prior to the real-time optimization also present some uncertainties. All of these uncertainties (particularly the uncertainties regarding measurement and the variability of components) can be estimated and accounted for into a new proposed standardization (weighting) matrix for selective redirection of observed errors to sources of strong uncertainties. Classically, the principle is the following: the base qualities considered to be most uncertain thus have their estimated values more likely to deviate from their nominal value than others are.

In this scheme, a priori knowledge on that variability (resulting, in particular, from operations practice) is crucial because it determines the quality of the estimate of the absolute value for each component, with iso-prediction on the quality of the resulting blend. A more formal estimate based on optimum stochastic filtering with heuristics simplifying configuration was implemented in an independent module (TIMEL) at the Port Arthur refinery. It can take into account interactions among properties and different uncertainties related to the origin of measurements (online or laboratory analysers) while guaranteeing the same predictions in nominal context if there is no coupling between the estimated properties.

3.1 Control: Stability, uncertainties, and delays

ANAMEL uses the model described above and an optimization algorithm to compute the control law applied to the blender. The closed-loop connection of an optimization algorithm subject to constraints and of a model adaptation scheme leads to a complex system of interactions, the functioning of which must be guaranteed to be "robust" in the presence of noise and perturbations. The interactions take place along two main paths: *i)* the optimization algorithm defining the control uses the model to predict the effects of the variations being considered, *ii)* the application of that control produces effects that are interpreted in order to adapt the model. There may be ambiguity in that interpretation, and the feedback loop that is created in this way may lead to instabilities. By using a carefully chosen Lyapunov function, convergence toward a zone where the success of the blend is guaranteed is proven. The proof is based on the analysis of the conditions for stationarity of the metric, and the property of convergence is obtained thanks to the specific choice of the law for adaptation of the model. The blends that are carried out are often impacted by delays (see Barraud (2006)), depending on the topology of pipes creating the blending network. This may have several sources, including delays in measurement and hydraulic delays. They decrease performances, cause oscillations in the closed-loop response (with the risk of destabilizing the system), and lead to the use of production margins, thereby generating excess quality costs. Compared to other control systems, one unusual feature of the blending problem is that the delays are not constant.

The variability in measurement delays is related to sampling and analysis methods. The delay value is known only *a posteriori*. In order to make the optimization algorithm robust against this uncertainty, results of asymptotic stability of discrete variables systems are used, representing the dynamic of the controlled blend, which are obtained by adaptation of space of states. Hydraulic delays are variable when ANAMEL changes the blend recipe (Barraud (2006)). Major, relatively uncertain delays can be compensated (see e.g. Bekiaris-Liberis and Krstic (2013c,b,a); Bresch-Pietri et al. (2014b, 2015, 2012a) and references therein) to some extent, but variable hydraulic delays require specific studies (Petit et al. (1997)). If variability is sufficiently slow, the structure of the error equation can be identified to a Halanay inequality (Bresch-Pietri et al. (2012b); Halanay (1966); Bresch-Pietri et al. (2014a)). This inequality establishes a bound for the solution of a differential inequality with variable delay. It provides the keys to controlling the arrangement by an inverse correspondence. Current studies relate to non-covered cases in which the delays are quickly varying, and important in the optimisation phase itself (Clerget et al. (2016a, 2017, 2016b)). By generally applying this approach, networks with pre-blends are being tackled, allowing an extension toward real-time multi- unit optimization of the RTDO (Real Time Dynamic Optimization) type, in which it is vital to control these dynamic aspects with variable delays.

3.2 Optimizing recipes and variable delays

To adjust blend recipes during production, periodic optimization of one quadratic criterion subject to affine constraints was introduced into ANAMEL back in 2001. In 2007, to control a batch blender for diesel hydro-desulfurization in the context of stricter sulfur specifications (when the target moved from 50 to 10 ppm), a mechanism for recording variable delays on several levels was developed and implemented in the system to integrate specific aspects of the line-up topology and incoming flows upstream of the specific blender, which operated continuously. In recent years, further developments of multi-criteria optimizations have been proposed with an arrangement combining targets for the recipes (to come as close as possible to a recipe based on a pre-established reference) and targets for the controlled properties (minimizing excess quality). New criteria relating to throughput targets were added to avoid certain dead-locks resulting from antagonistic hydraulic constraints. An economic component linked to the cumulative cost of the recipe is added to those technical criteria.

3.3 Automated injection of additives

For certain properties to be controlled, regulatory requirements are too strict to be achieved simply by blending existing bases produced in the refinery. That is the case, for example, for certain cold-resistance properties of diesels such as targets for the Cold Filter Plugging Point (CFPP), or cetane index. They are thus obtained by injecting very small quantities (several hundred ppm) of specific chemical additives (the dope) upstream of the blend. This is a finicky step because the response of fuels to the injection of additives is generally non-linear and poorly understood, at least for the time being. So, it is common practice in the profession to set a fixed volume of dope to incorporate in order to improve a given property. As a major improvement in our integrated solution, a regulation system based on an internal model controller made possible to adjust the incorporation of the dope in a fine-grained, gradual way.

This regulation, which is done at the same time as the optimized adjustment of the blend recipe, is based on a dope reactivity model with variable gain and variable delays. This dynamic model is created for each additive based on response curves from laboratory experiments conducted in our technical centers, supplemented by sensitivity curves from suppliers. When controlling the diesel CFPP, the experimental protocol used for the on-line measurements causes, for structural reasons, uncertainties in dating that can disrupt the controller. The measurement is in fact intermittent with a delay that ranges from 20 to 45 minutes; the delay is a function of the number of sequential analyses needed to progressively decrease the temperature up to the point at which the filter clogs, which is how

CFPP is measured. To limit the incorporation of these expensive additives, work began in 2015 to improve the synchronization mechanism in the context of prolonged, intermittent measurement with uncertain dating. By relaxing the convergence speed, the new algorithm that has been established offers convergence that can be explicitly guaranteed over a broad modeling error range, even when there are uncertainties (sometimes major) in the dating of measurements. This analysis contains, in an innovative form, the work on robustness against measurement delays which is mentioned above. Implementation in the refinery has been done, successfully, in 2016.

4. CONCLUSION

We have offered some perspectives on the work done in recent years, both in the technical area of interoperability in new automation environments and industrial computing, and in the scientific area related to estimation, control, and optimization for periodic adjustment of the recipes used to produce commercial fuels. Progress of this kind is important in a context of increasingly complex perturbations and operating constraints. The benefits of this integrated solution are related to lower costs for scalable services and maintenance for suppliers (Leuna) and to gains from implementation of the integrated optimization in the automation of the gasoline blender (Port Arthur). Those cumulative gains at the two refineries exceed 2 million USD per year. Future work will relate to the introduction of robust approaches providing greater mastery of uncertainties and to increasingly ambitious optimization of more broad-based production, in order to integrate complete production lines (diesel line and gasoline line), synchronizing several interconnected processing units.

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