PLANTWIDE ECONOMICAL DYNAMIC OPTIMIZATION: APPLICATION ON A BOREALIS BORSTAR PROCESS MODEL

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Abstract: A novel plantwide dynamic optimizer PathFinder has been applied to a dynamic model of a Borealis Borstar process. PathFinder optimizes dynamic paths subject to a merely economical criterion. Introduction of process constraints allows for a gradual migration from the currently used transition towards a more optimal transition. Special care has been taken to integrate the optimizer with on-line control tools. The results show a significant improvement in added value during a grade transition.

Keywords: Plantwide, Optimal trajectory, Optimization, Grade Transition, Chemical industry

1. INTRODUCTION

The chemical process industry is facing a huge problem to increase their capital productivity. A solution to this problem is demand driven process operation. This implies that exactly these products can be produced that have market demand and take price advantage of a scarce market. Flexible operation of production is therefore required [Backx, *et al.*, 1998].

A new integrated process control and transition optimization technology is needed for this purpose.

The idea of optimization of grade transitions has been introduced by McAuley [McAuley and MacGregor, 1992]. Based on rigorous dynamic models optimal open-loop paths are calculated. The cost function has been improved into a more straightforward economical framework [Van der Schot et al, 1999]. The introduction of an economic objective function introduces strong non-linearities resulting in a strong increase in model evaluations. Special effort is paid to reduce the number of model evaluations to make the optimization feasible within a realistic timeframe. The PathFinder rigorous model based dynamic optimizer has been developed for these purposes. An application on a Borealis Borstar process is discussed. The paper is organized along the following four Sections:

- In Section 2 the formulation of the plantwide economic optimization criterion is given.
- Subsequently, in Section 3 a framework for on-line implementation of the optimized paths is discussed.
- In Section 4 relevant aspects of the Borstar process are described.
- Finally, Section 5 describes the application of PathFinder on a Borealis Borstar process.

2. PLANTWIDE DYNAMICAL ECONOMICAL OPTIMIZATION

PathFinder is a generic framework for plantwide economical dynamic optimization.

An economical balance is being calculated for the entire process over a finite time horizon. For this purpose the revenues and costs are assigned to various economical flows entering and leaving the process (Figure 1).

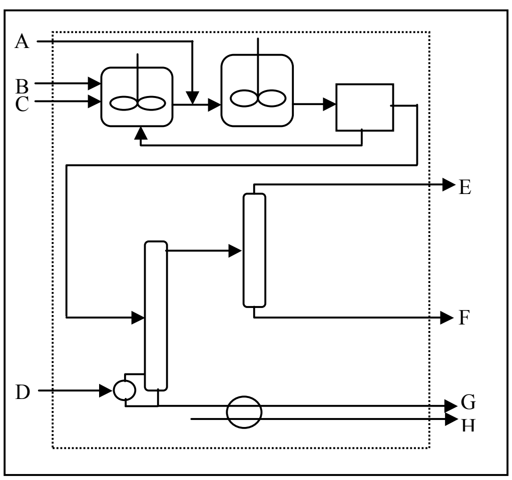

Figure 1 Example of the Generic Plantwide Economic Process Framework

In general, three types of flows characterize a process:

- Economical flows that are consumed by the process. In most cases these will correspond to the use of raw material (Figure 1, flow A, B and C), but also the use of utilities (cooling water, steam (Figure 1, flow D), electricity…) can be accounted for as well. These flows are characterized by a fixed price per unit consumption.

- Economical flows that are generated by the process, under a fixed price condition per generated unit. Typical examples are material flows of reaction side products that can be sold but where the quality of the generated product is not determined fully inside the process (Figure 1, flow G). The price can be negative if side products result that must be reworked afterwards as waste material. Also non-material flows such as generated steam (Figure 1, flow H) or electricity can be accounted for in the same fashion.

- Economical flows corresponding to material or energy flows where the generated value depends on the value of a set of quality variables. Typical examples are reaction end products that must comply with given customers requirements, distillation tower top and bottom products that must satisfy purity demands (Figure 1, flow E and F) …

It is key for an economical framework that the prices that must be accounted for in the last class of economical flows have a discrete nature. Products meeting a set of specifications have high economical value, while products that are outside the specification range ('off spec') show a value drop.

As such, the economic criterion to be optimized is given by the added value over a fixed time horizon T.

$$
\begin{aligned}
& AddedValue = \\
& -\int_0^T \sum_i^L Inflow_i(t)\, price_i\, dt \\
& +\int_0^T \sum_i^M Outflow_i(t)\, price_i\, dt \\
& +\int_0^T \sum_i^N Productflow_i(t)\, price_i(QPar_1(t), QPar_2(t), \ldots)\, dt
\end{aligned}
$$

Within PathFinder various specifications (also called 'grades') can be introduced for each of the existing product flows (Figure 2). A grade consists of a set of quality parameters, which form bounded regions by the introduction of inequalities.

Based on the given economical criterion, one can calculate improved dynamical paths to move from one operation point to another. As such it can be used to calculate economically optimal grade changes, production load changes, start-up and shut down procedures…

Economically optimal grade change trajectories reduce the transition cost and thus make it easier to operate the process in accordance with market demand. It also enables a flexible process operation strategy that is no longer coupled to a fixed grade slate, but that allows shortcuts between most of the grades in the grade slate.

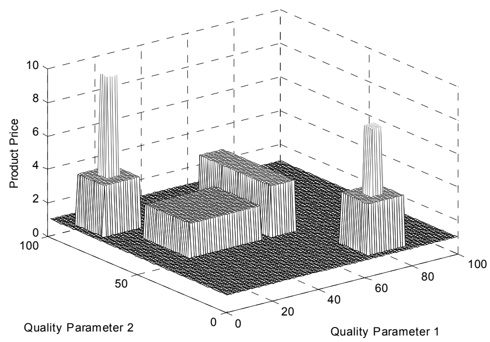

Figure 2 PathFinder's multigrade set-up

It can readily be understood that this economic formulation leads to different optimal trajectories if the market conditions change from an unsaturated market condition towards a closed market. In an unsaturated market raw material and utility consumption will be less penalized since the on-spec product will typically generate significantly more benefits compared to the production costs. On the other hand, in a closed market, the optimizer will automatically strive for cost reduction, since the on-off spec price difference will not be as large.

The optimizer searches for the optimal process manipulations, such that the resulting trajectory is economically optimal. It is clear that a dynamic process model is needed to enable the calculation of the Added Value given the applied process manipulations. The nonlinear dynamic model equations (set of DAE's) have to be integrated over the time horizon given by the input manipulations.

Constraints are added to the optimization problem, restricting the optimization freedom.

The reasons for the introduction of these constraints (Path Constraints and Rate of Change constraints on MV's and CV's) are:

- Guarantee a safe and feasible operation during the transition.

- Constrain the optimizer freedom such that the new trajectory doesn't differ too much from the initial trajectory.

The last reason is important when one has no blindfolded confidence in the process model. Adding constraints will allow one to migrate gradually from a well-known recipe to a new recipe.

PathFinder is a robust and fast solution for the above optimization problem. Though the objective function is strongly non-linear, due to the discontinuous price function, typically 5 up to 10 trajectory simulations and model linearizations are needed for the cases that have been analyzed (compared to 500 up to 1000 model evaluations with a SQP optimization scheme). These model evaluations are the bottleneck for a faster calculation time. In [Van Brempt, *et al.*, 2001] relevant implementation topics are discussed.

3. INTEGRATED TRAJECTORY CONTROL AND OPTIMIZATION TECHNOLOGY

The manifest reduction that has been achieved in the number of required model evaluations, makes *off-line* economical plantwide dynamical optimization feasible. However, given the currently available computing power, *on-line* economical plantwide dynamical optimization will not be feasible for most industrial problems.

Therefore, a general framework has been set up in order to cope with the challenge to integrate dynamic optimization and on-line control [Van Brempt, *et al.*, 2000]. The key idea is explained in *Figure 3*.

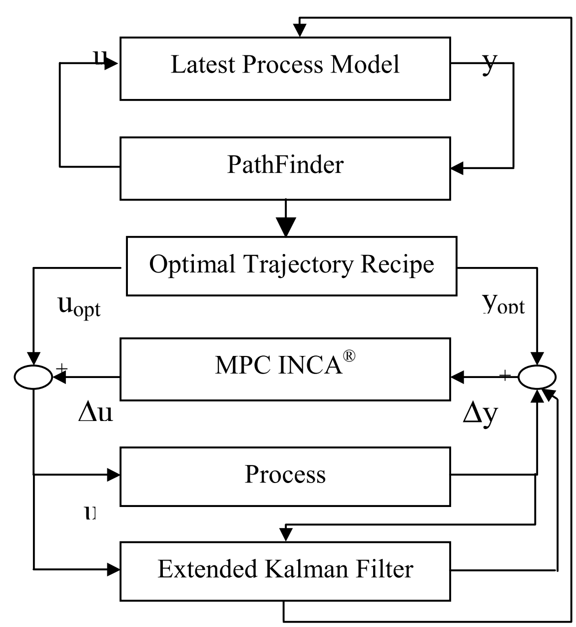

Figure 3 Integration of MPC control technology and optimization technology

PathFinder calculates off-line optimal dynamic economically paths based on the non-linear rigorous dynamic process model. These manipulated and controlled variable trajectories are as such applied to the process. The on-line controller corrects only for the deviations Δu and Δy ('delta mode') from the process input-output setpoints u_{opt} and y_{opt} that are given by the optimizer. These deviations will occur due to model-plant mismatch and due to disturbances entering the process.

The delta-mode guarantees a best of both worlds operation. The trajectory has generally been carefully designed with the knowledge of the non-linear process. It would be a pity to have this result overridden by a linear model controller. Therefore this trajectory is applied as such to the process. It puts a curb onto the controller, and the controller is allowed to shift the deviations of the input-output trajectory (u_{opt}, y_{opt}) between the controller input and output. It does not only try to follow as closely the output trajectory, but makes a compromise between deviations from the output trajectory and from the input trajectory.

As explained in the previous section, the long trajectory simulation time determines the optimization calculation time. In practice the optimizer will therefore still need a considerable time to calculate a new trajectory. Therefore PathFinder is started some time before the trajectory has to be initiated, with up-to-date market conditions that can be uploaded from an ERP environment.

In order to reduce plant-model mismatch, PathFinder will use the latest instance of the rigorous model that is known, with the latest state updates in case an Extended Kalman Filter is available. Once the optimal trajectory is calculated and acknowledged, it is sent to the controller environment (*Figure 3*).

4. THE BORSTAR PROCESS

Development in polymer materials is nowadays geared towards increased strength, resulting in less thickness for films, pipe and container walls. This results in a clear reduction in weight, transport cost and material usage, as such giving less harm to the environment.
Less taste and odor is also an issue for polymer materials, as is the speed of processing the polymer materials, which allows faster production for end user applications. This requires more tailoring of the molecules. A bimodal molecular weight distribution is often used as it is a tailored distribution of the incorporation of co-monomers. Figure 4 shows how end polymer properties are affected by the molecular weight of the polymer molecules.

There are basically two routes to tailor-make a polymer; either to tailor the catalyst used in the production of the polymer and/or tailor the polymerization process. Both routes are extensively used. The following description will describe the up-to-date approach of modifying the polymer by the process route.

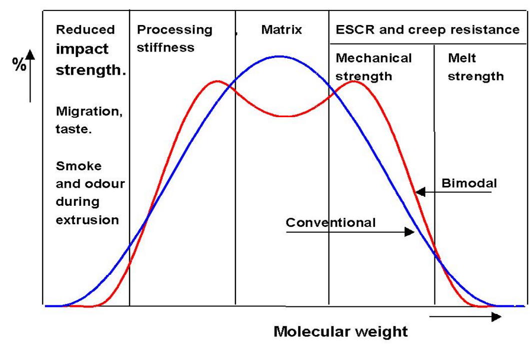

Figure 4 Molecular weight distribution can be more easily adapted with bimodal than uni-modal materials to meet the property needs of the end application.

The polymer that is being produced depends not merely on the kinetic properties of the catalyst, but also on the temperature, pressure and duration of polymerization as well as on the concentration of the polymer and monomer involved in the reactions. The polymerization process used to produce the material controls the latter. There have been strong developments in this field to enable wide variations in the properties of the final polymer. Figure 5 shows the process for producing bimodal molecular weight distributed polymer as well as wide variation in co-polymer incorporation.

The Borstar process consists of at least three reactors. One pre-polymerization reactor is used to start the catalytic polymerization process in a controlled manner as well as developing the desired particle morphology. The subsequent loop reactor produces the low molecular weight polymer. Propane is used as the diluent. Operating the reactor above the critical thermodynamic point gives a very low solubility of PE in the diluent. The probability of fouling is hence greatly reduced compared with process using other diluent. The loop reactor can therefore produce polymer with larger variation in density than a number of other processes. The high molecular weight part of the polymer is produced in the fluidized bed reactor following the loop reactor.

An extra versatility of the combined Borstar process comes also with the ease of varying the co-monomer content in each reactor and thereby tailor-making the co-monomer distribution of the final polymer. Various polyethylene grades can be produced on the same process using a carefully chosen set of flow, temperature and pressure setpoints (SPi) that we will refer to as a "recipe". A given polyethylene grade will be characterized by a specified density and melt index.

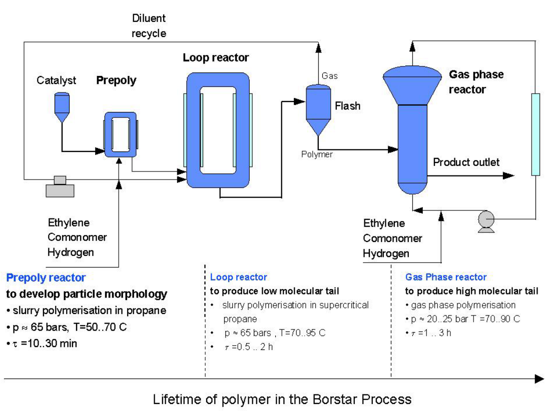

Figure 5. The Borstar process for producing bimodal MWD polymer as well as variation in co-polymer distribution.

When changing from one polymer grade to another polymer grade, setpoints must be moved from one recipe to the other, driving the process through a zone where off-specification product is made. Typically the transition path for recipe setpoints will be selected to minimize production of low value off-spec product.
Borealis developed a rigorous dynamic model for the Borstar process. This model is used to demonstrate the application of PathFinder.

5. APPLICATION OF PATHFINDER ON THE BORSTAR PROCESS

PathFinder's optimization technology is applied on a model of the Borstar process in order to optimize the transition from one specific polymer grade to another grade.
In *Figure 6* optimized trajectories are shown for both quality variables. Notice that in both situations the off-spec time has considerably been shortened to about a half of the original off-spec time. Also observe that the optimizer fully exploits the dynamical behavior of the process within the freedom of the entire specification band to optimize the transition. A typical optimizer behavior results for the density variable: the process first moves away from the desired spec, changes direction within the specification band, and takes full speed to go to the other grade. Upon arriving in the second grade specification, the process enters with full speed into the specification zone, bumps against the opposite boundary, and swings back without leaving the specification boundary.

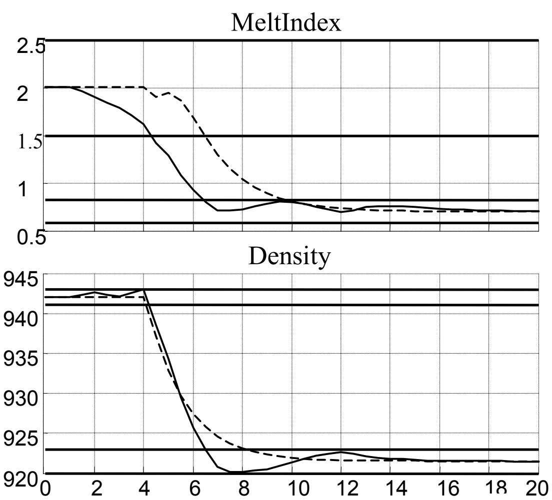

Figure 6 Trajectories for quality variables Density and Melt Index (together with specification boundaries): initial trajectory (--- , final trajectory (solid).

In *Figure 7* some MV trajectories are shown. The production setpoint controls the ethylene inflow using a PI controller. One can easily notice the move times in the trajectories, i.e. the timestamps where the optimizer is allowed to change the MV values. In between these values, the MV values are kept constant. In total an optimization problem with 174 move times (degrees of freedom) was solved. Observe also that the original trajectory was a rather quasi steady state transition, while the new trajectories are fully dynamic.

In *Figure 8* the economical added value is shown in function of time. During Off-Spec the added value drops due to the fact that only a lower price can be achieved for the end product. The optimized trajectory shows a much shorter dip due to the fact that the off-spec time is shortened considerably.

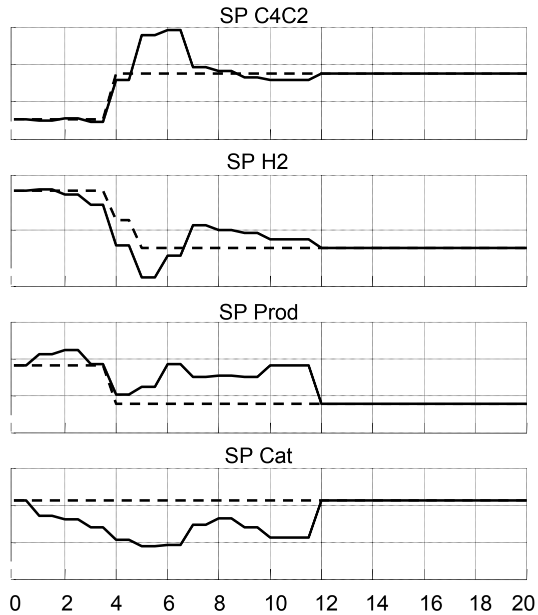

Figure 7 Manipulated Variable Trajectories (initial trajectory (---), Optimized (solid)).

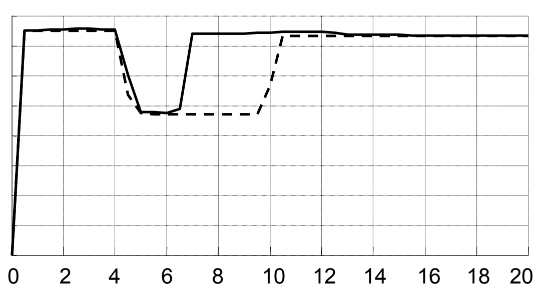

Figure 8 Added value: initial trajectory (---), optimized (solid).

6. CONCLUSION

A plant wide dynamical optimization tool has been developed for optimization of a straightforward economical criterion. Several types of constraints can be introduced, such that a safe operation can always be guaranteed and such that a gradual migration from a known recipe to a renewed recipe is obtained.

PathFinder has especially been laid out to increase optimization speed by limiting the number of necessary model evaluations. The optimizer is seamlessly integrated with a model predictive control technology such that on-line implementation of the optimized paths becomes feasible.

PathFinder has been successfully applied on a grade transition problem for the Borstar process. The results showed considerable shortening of the off-spec time as well as a reduction of the overall cost of a grade transition.

7. ACKNOWLEDGEMENTS

This work is supported by the European Community project polyPROMS (GRD1-2000-25555): Development of Advanced Polymerization Process Modeling, Simulation, Design and Optimization Tools. The scientific responsibility is assumed by its authors.

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