ECONOMICALLY OPTIMAL GRADE CHANGE TRAJECTORIES: APPLICATION ON A DOW POLYSTYRENE PROCESS MODEL

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Abstract: A novel dynamic optimizer PathFinder has been applied to a dynamic model of a Dow polystyrene production facility at Tessenderlo, Belgium. PathFinder optimizes grade transitions subject to an economic cost function, taking into account the raw materials' prices and different price settings for on-spec and off-spec product. 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 restrict the number of required model simulations, in order to avoid large optimization times. The results show a significant improvement in added value during a grade transition.

Keywords: Predictive control, 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. A very important requirement for this technology is to enable the calculations of grade transitions such that these transitions become feasible and economically attractive.

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 DOW polystyrene production facility is discussed.

The paper is organized along the following four Sections:

- In Section 2 the formulation of an economic optimization criterion is given. It is shown that a standard optimization algorithm would be very time consuming.
- Subsequently, in Section 3 a framework for integration of trajectory control and trajectory optimization is explained.
- In Section 4 relevant aspects of the polystyrene solution process are described.
- Finally, Section 5 describes the application of PathFinder on a Dow polystyrene production facility at Tessenderlo, Belgium.

2. ECONOMICAL OPTIMIZATION CRITERION

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.

Since the incentive for the elaboration of optimal grade changes is merely economical, it is reflected in an economically driven optimization criterion (Eq. 1). The goal is to maximize added value (AV) during a time horizon T while making the transition from one grade to another grade [Van der Schot, *et al.*, 1999].

$$AV(T) = \int_0^T price(t)throughput(t)dt - \int_0^T \sum_i feed_i(t)\cos t_i(t)dt + holdup(T)price(T) - holdup(0)price(0) \qquad (1)$$

The first term accounts for the benefits gained during the trajectory by producing the desired end-product. It depends on the production throughput and is a highly non-linear function with regard to product price (*Figure 1*). The high non-linearity arises from the fact that mostly a good price is paid for on-spec material, while the market price for wide-spec or off-spec material is significantly lower. Although integration softens the non-linearity, it remains nevertheless very severe. The specifications are typically expressed in terms of product properties, which are themselves non-linear (dynamic) functions of the process conditions.

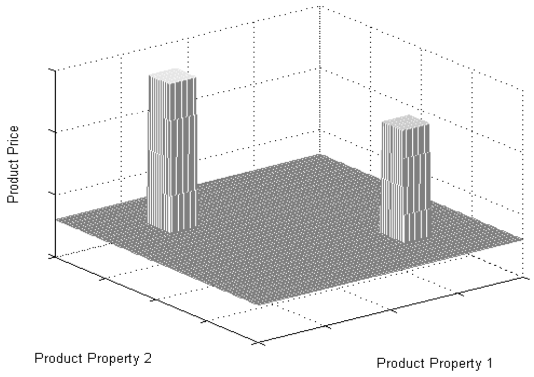

Figure 1 Product Property Price Function

The second term in (Eq.1) accounts for the economic costs of all the feed stock materials and cost of plant operation. The final two terms make the bookkeeping of process material holdup at the initial and final time instant. This term is included in order to avoid the optimizer to clear the reactor at the end of the trajectory to gain extra income.
It can readily be understood that this formulation leads to different optimal trajectories if the market conditions change for either the feed products either the end-product.

The optimizer searches for the optimal process manipulations, such that the resulting trajectory is economically optimal. The relation between optimization parameters, the process and the economic cost is shown in *Figure 2*.

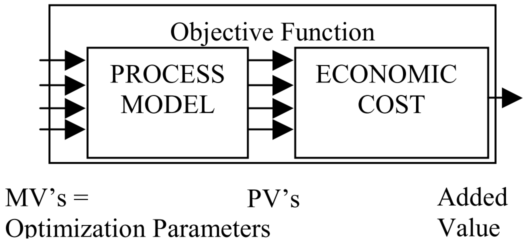

Figure 2 Relation between Manipulated Variables (MV's), Process Variables (PV's) (such as flows, product properties, holdups…) and Added Value for the original configuration

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 optimizer, which restrict the optimization freedom.

- End-point constraints on CV's
- Path constraints on CV's
- Input constraints (absolute boundaries and rate of change constraints) on MV's.

The reasons for the introduction of these constraints are:

- Guarantee a safe and feasible operation during the transition.
- Guarantee that the desired product properties and production level are achieved after 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 slowly from a well-known recipe to a new recipe.

Apart from the constraints, other handles are available to steer the optimizer:

- Selection of manipulated variables (MV's)
- Selection of move times for the MV's
- Introduction of weights that encourage the use of some MV's over other MV's
- Introduction of weights that penalize constraint violation more for some CV's over other CV's

PathFinder is a robust and fast solution for the above optimization problem. Though the objective function is strongly non-linear, 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

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

PathFinder calculates off-line dynamic economically optimal grade change recipes. These manipulated and controlled variable trajectories are as such applied to the process. The controller only corrects 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.

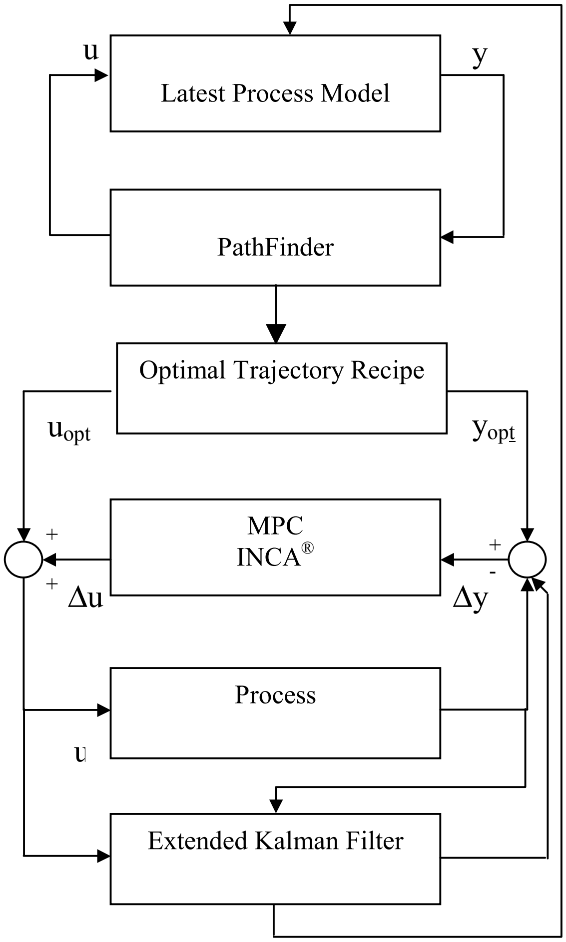

Figure 3 Integration of MPC control technology and optimization technology

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 several hours to calculate a new trajectory. Therefore PathFinder is started several hours before the trajectory has to be initiated, with up-to-date market conditions. 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. The initial trajectory for PathFinder could either be a previous best-practice trajectory, either a previous PathFinder result (under different market conditions).
Once the optimal trajectory is calculated and acknowledged, it is sent to the controller environment (*Figure 3*).

4. THE POLYSTYRENE SOLUTION PROCESS

Polystyrene is mostly produced using a solution process. A simplified layout of a typical polystyrene solution process can be found in Figure 4.

The process consists of a combination of several plug flow reactors. Styrene, a solvent and in some cases an initiator are fed to the first reactor. Reactors are usually operated at sequentially higher temperatures with a final conversion at 60-90%. Unreacted monomer and the solvent are separated from the polymer under vacuum. The hot melt is then pelletized while the monomer and solvent are condensed and recycled. Additives may be added at different places in the process.

Various polystyrene 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 polystyrene grade will be characterized by a set of properties (PROPj).

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.
Dow developed a rigorous dynamic model for the specific process used for the production of polystyrene at Tessenderlo, Belgium. This validated model is used to demonstrate the application of the INCA® controller to a polystyrene process.

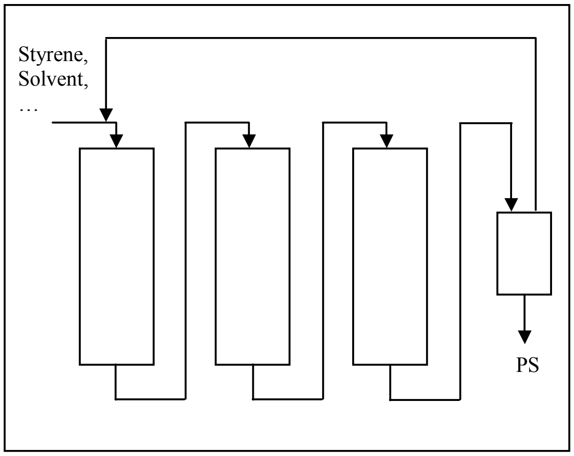

Figure 4 Schematic description of a typical solution polystyrene process

5. APPLICATION OF PATHFINDER ON THE DOW POLYSTYRENE PROCESS

PathFinder’s optimization technology is applied on a model of the Dow polystyrene production facility at Tessenderlo, Belgium.

Fourteen variables were used as MV’s for PathFinder including setpoints for temperatures and flows, for the reaction as well as for the separation sections of the process. For each variable 13 move times were defined, resulting in 182 degrees of freedom for the optimizer. Path constraints are applied on 8 process variables, rate of change constraints on 10 MV’s and absolute upper and lower boundaries on all 14 MV’s.

Optimal trajectories were subsequently calculated for two different market situations depending on the price of off-grade product (Table 1). Indeed, off-grade product can be used in low-end applications and its price is therefore subject to offer and demand fluctuations. Both market situations are characterized by a considerable difference between the on-spec and off-spec material price. In the first case off-spec material represents a serious loss compared to the raw material, while in the second case off-spec material can be sold with a benefit compared to the monomer that is being used.

Price	Case 1	Case 2
Onspec - Offspec	High	Low
Offspec - Styrene	negative	positive

Table 1. Two different market situations with respect to the relative prices of on-spec material, off-spec material and monomer.

In *Figure 5* optimized trajectories are shown for both situations. PathFinder started from a trajectory that was given by Dow. The initial trajectory shows first a production decrease, followed by a transition from one grade to another grade.

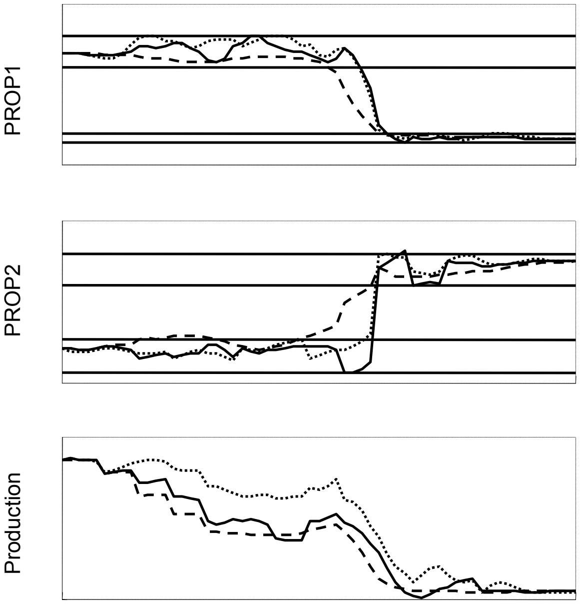

Figure 5 Trajectories for quality variables PROP1 and PROP2 (together with specification boundaries) and for production rate for three cases: initial trajectory (---), Case 1 (solid) and Case 2 (...).

Notice that in both situations the off-spec time has considerably been shortened to about one quarter 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 is shown: 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.
Also remark that in both cases production has been increased while being in the original grade. The production has been increased more in the second case, since the off-spec is not penalized as much as in the first case.

In *Figure 6* some MV trajectories are shown. 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. Observe also that the original trajectory was a rather quasi steady state transition, while the new trajectories are fully dynamic.

The reactor feed flow (MV2) is obviously manipulated and related to the production increase observed in *Figure 5*. The rapid change of MV3 is responsible for the fast clipping of the PROP2 value. If this brusque change of the value of MV3 would be unacceptable for some reasons, it could be limited by introducing a proper rate of change constraint. Other MV moves would typically look like the one shown here for MV1.

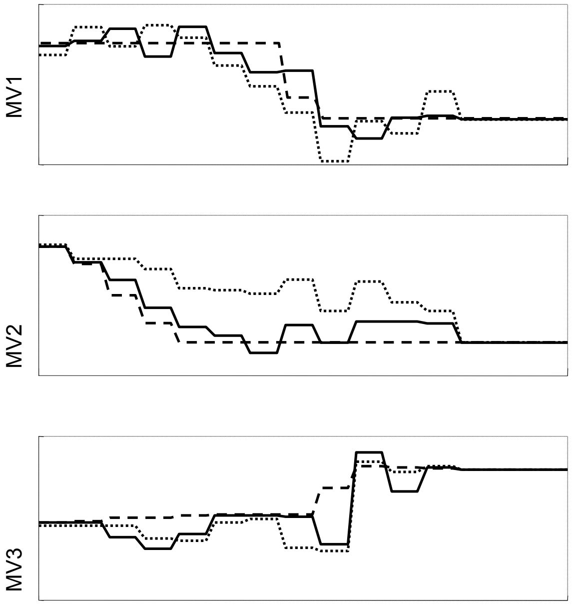

Figure 6 Trajectories for three selected MV's for three cases: initial trajectory (---), Case 1 (solid) and Case 2 (...).

In *Figure 7* a path constraint (PC1) is shown that was imposed on a specific process variable known as a constraint: operating beyond that point would lead to undesirable effects. Notice that the optimizer pushes the process against this boundary to increase profit.

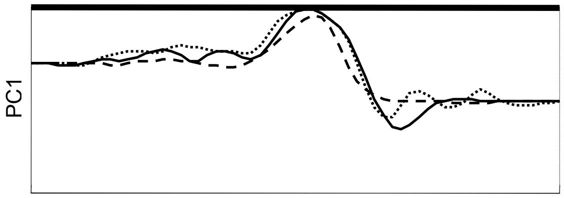

Figure 7 Trajectory for a constrained process variable for three cases: initial trajectory (---), Case 1 (solid) and Case 2 (…). The thick solid line corresponds to the upper boundary that is imposed on this variable.

6. CONCLUSION

A robust optimization technology PathFinder for the calculation of economical optimal grade change trajectories has been presented. It is seamlessly integrated with a model predictive control technology such that controlled (optimal) grade transitions are straightforward.

PathFinder derives dynamic grade change-over trajectories that optimize added value, given the economic price settings for the raw materials and end-products. Several types of constraints can be entered, 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.

PathFinder has been successfully applied on a dynamic model of a Dow polystyrene production facility at Tessenderlo, Belgium. Two different market conditions were analyzed. 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

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