OPTIMAL TRAJECTORIES FOR GRADE CHANGE CONTROL: APPLICATION ON A POLYETHYLENE GAS PHASE REACTOR

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Abstract: This paper describes the development of a Grade Transition optimizer PathFinder® that enables a high performance demand driven operation in the chemical process industry. The technology makes use of a dynamical rigorous model based optimization of an economic criterion along a grade change trajectory. An application on a large grade slate for a polyethylene gasphase reactor is discussed.

Keywords: Optimal trajectory, Optimization Problems, Chemical industry, Plantwide

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. A flexible production operation is therefore required.

A new process control 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.
PathFinder® rigorous model based dynamic optimizer has been developed for these purposes. An application on a polyethylene gasphase reactor is discussed.

The paper is organized along the following four Sections:

- In Section 2 the economic incentive for grade transition optimization is explained.
- Subsequently, in Section 3 the formulation of an economic optimization criterion is given. It is shown that a standard implementation would be very time consuming.
- In Section 4 implementation aspects of PathFinder® are given into more detail.
- Finally, Section 5 describes the application of PathFinder® on a fluidized bed gas phase high density polyethylene (HDPE) reactor.

2. ECONOMIC BACKGROUND

Nowadays chemical processing industries are facing a tremendous pressure to improve their capital productivity. Some possible explanations for this evolution are the global competition, the worldwide saturation of markets and the tightening of legislation on ecosphere loads and resource consumption.

The answer by most of the chemical industries to these problems is a predominantly **supply driven** process operation that focuses on minimization of operation cost. This is realized by an increase of scale and by minimization of the number of product types per production site.

As a direct consequence plants only operate a limited number of product types. Typically a largely fixed product slate is followed with recipe driven product changeovers.

However, a constrained market situation asks for a **demand driven** mode of process operation, requiring flexible processing of different feedstocks to produce a flexible set of end-products [Backx, *et al*., 1998, plenary ton in PISA!!!!]. This implies that exactly these products can be produced that have market demand and that take advantage of scarceness in the market of specific products at each moment.

Since the right product can be produced at the right time in a demand driven process operation, capital blocked in stored products and intermediates is minimized. A shortened production-to-product delivery cycle also increases capital turnaround. Each of the mentioned effects directly contributes to an increase of capital productivity.

A general framework has been set up in order to cope with these challenges [Van Brempt, *et al*., 2000]. In this paper special attention will be paid towards the calculation of optimal input-output trajectories for grade change control.

Optimal grade change trajectories will reduce the transition cost and thus make it economically more attractive to switch the process to a more profitable operation point. It also enables a flexible process operation strategy that is no longer coupled to a fixed grade slate, but that allows shortcuts between two arbitrary grades in the grade slate.

3. ECONOMICAL OPTIMIZATION CRITERION

As explained before, the incentive for the elaboration of optimal grade changes is merely economical. This is reflected in an economically driven optimization criterion (Eq. 1), where 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. The high non-linearity arises from the fact that only a reasonable price is paid for on-spec material, while off-spec material is less worthy or could even cost money. The specifications are typically expressed in terms of (one or several) product properties, which are themselves non-linear (dynamic) functions of the process conditions (Fig. *1*).

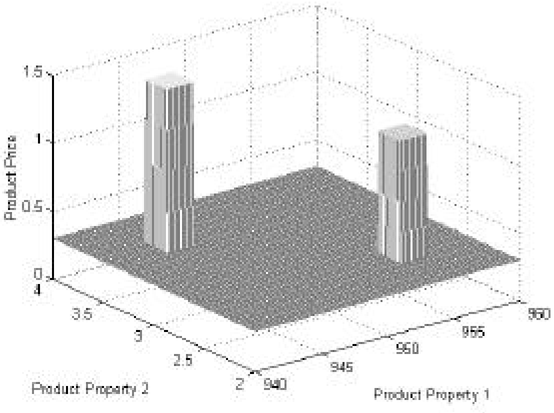


Fig. 1 Product Property Price Function

The second term in (Eq.1) accounts for the economic costs of all the feed flows to the process. 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 (***Fig. 2***).

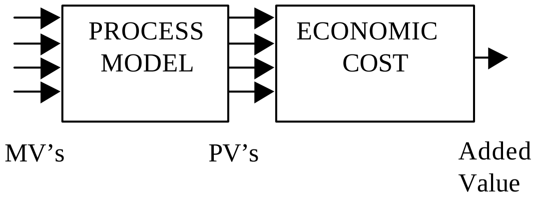


Fig. 2 Relation between Manipulated Variables (MV's), Process Variables (PV's) (such as flows, product properties, holdups…) and Added Value.

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.

Apart from the optimization criterion constraints are added to the optimizer. End-point constraints guarantee that the desired product properties and production level are achieved after the transition. Path constraints guarantee a safe operation during the transition. Input constraints restrict the free use of optimization parameters (MV's).

Two particular aspects make this optimization a real challenge:

- For the calculation of the economic cost, a dynamic process model simulation over the given time horizon is needed. This model simulation is typically very time expensive, ranging from 1 minute to several hours for one simulation run.
- The highly nonlinear objective function typically results in a lot of function evaluations needed by the optimizer.

In order to avoid a very time consuming optimization run, modifications are made to the standard optimization schemes, as explained in Section 4.

4. IMPLEMENTATION ASPECTS

PathFinder® is a robust and fast solution for this optimization problem. In this section three relevant implementation topics are discussed: an optimization formulation that aims at reducing computation time (SSQP), some parameterization topics and selection of the model simulation time horizon.

4.1. SSQP

A closer look at the optimization problem learns that the high computation time arises from the combination of a highly nonlinear economic cost function with a computational intensive model simulation. However, the calculation time of the economic cost function itself is very fast. On the other hand, the process model is usually very linear compared to the economic criterion.
The idea is therefor to split up the optimization scheme into two levels [Van der Schot, *et al.*, 1999](Fig. 3).

At a lower level a constrained optimization problem is solved (SQP) based on a linear approximation of the process model around the initial trajectory and the nonlinear economical criterion. This optimization runs at high speed since no rigorous model evaluations are needed.

Several commercial dynamic modeling tools (gPROMS, SpeedUp, Simulink…) provide ways to extract linear models or DAE Jacobian information from the rigorous model at desired time instants.

At the higher level the lower level SQP optimization result is validated on the non-linear model. The high level optimization processes this result using a modified Trust Region approach.

The first step in this approach is to judge whether the new real result has improved. Therefor a merit function taking both Added Value improvement as constraint violations into account is defined. This merit function should be as consistent as possible with the lower level SQP merit function.

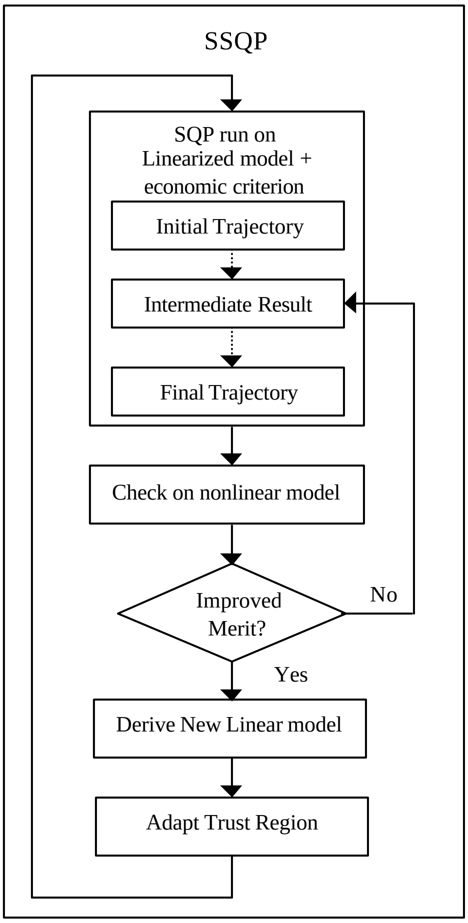


Fig. 3. SSQP and modified Trust Region architecture

If the new real trajectory has a better merit than the previous one, it is selected as a new starting point for a subsequent low level SQP run after a new linear model has been derived around the new trajectory.

If the real merit function is worse, a new trajectory is chosen from the list of all intermediate gradient evaluations in the lower level SQP. A possible way is to look for the best merit in the halved list. Rather than performing a line search between the original trajectory and the disapproved trajectory, the use of this list is more likely to go about an infeasible region. In a traditional Trust Region approach a way to handle worse real solutions is to limit the optimization input freedom and to start another SQP optimization from the original trajectory. In this case however it turns out to be an inefficient handle, since in most cases the same or a shortened list as before comes out.

The second step in this approach is to alter the Trust Region. The Trust Region is the region where the inputs are allowed to vary (combined with the hard input constraints). If the improvement predicted based on the linear model is very similar as the one based on the non-linear model, the Trust Region of the linear model can be increased. On the other hand, if the prediction is bad, the Trust Region should be reduced such that the optimizer can only use the linear model locally.

Unlike the traditional methods, the decision to alter this Trust Region is uncoupled from the decision to accept a solution.

4.2. Optimization Parameterizations

Actually three parameterizations play a role in this scheme.

- Input parameterization. The inputs are only allowed to change at well defined time stamps, and are maintained in a zero order hold between the time stamps.
- Linear Model time stamps. Only at well defined time stamps along the trajectory, linear models are derived. These time stamps should be chosen judiciously such that new linear models are mainly derived at the time nonlinear process variables change most.
- Output parameterization. The time stamps at which the simulation output is sampled determine the accuracy of the result.

4.3. Time Horizon

The time horizon during which the grade transition is simulated is taken such that after the last input move the process has the time to come to a steady state. As such unexpected transients after the simulation run are impossible.

4. APPLICATION: THE POLYETHYLENE GASPHASE REACTOR

The PathFinder® technology mentioned before is applied to a high-density polyethylene (HDPE) fluidized bed gas phase reactor. A complete rigorous dynamic model for the polyethylene gas phase reactor has been developed in *gPROMS*.

The process is depicted in Fig. 4. The ethylene monomer and butylene co-monomer react to HDPE. The unreacted ethylene goes to the top of the reactor and is recycled. The butylene/ethylene (CH_4/CH_2) ratio and the hydrogen/ethylene (H_2/CH_2) ratio are crucial handles to obtain HDPE with the desired density and melt-index (both quality parameters define the grade). Catalyst flow and pressure setpoint are relevant handles that govern the reactor production level. Nitrogen is used as a cooling and transportation medium and is inert for the reaction.
There are 3 PID-controllers embedded in the process: ethylene flow controlling total gascap pressure, coolant flow controlling bed temperature and a reactor level controller. Furthermore ratio controllers are implemented such that CH_4/CH_2 and H_2/CH_2 can be used as manipulated variables.

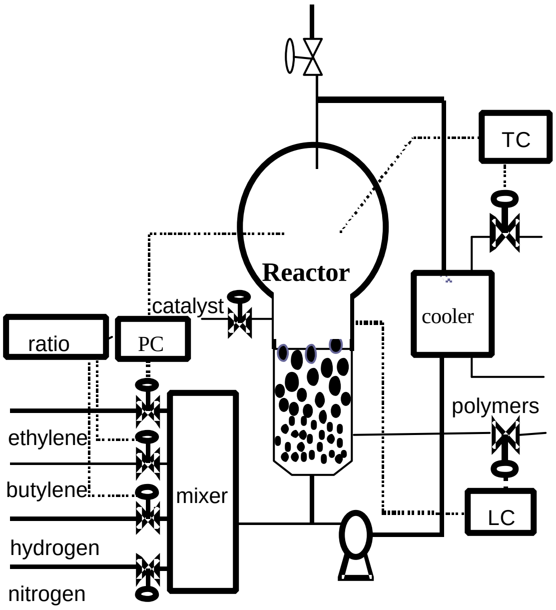


Fig. 4 Polyethylene Gasphase Reactor Process

Flexible operation of a HDPE-process implies the need for a technology that supports optimal grade change. PathFinder® rigorous model based dynamic optimizer provides a solution for this problem.

A fixed grade slate consisting of 19 transitions has been defined as a benchmark for this problem (Fig. 5). For each of these transitions an optimal trajectory has been calculated. Also some optimal short-cut trajectories have been calculated.

Pathfinder® uses four MV's as optimization handles: CH_4/CH_2, H_2/CH_2, Pressure Setpoint and Catalyst Flow. The optimizer needs the following PV's for calculation of the Added Value: feed flows, product flow, reactor holdup and quality parameters density and (logarithm of) melt index. A path constraint is introduced on the cooling water flow, in order to guarantee a safe operation. End point constraints are put on both product qualities (defining the new grade) and on the production level. Input constraints are put on all MV's.

Typically 10 up to 15 time stamps are used for the input moves, bringing the total number of optimization parameters to 40 up to 60. One model simulation takes on the average 1 minute, while the derivation of one set of linear models along the trajectory takes on the average 5 minutes.

As an initial trajectory the new steady state solution is applied at once. If cooling limitations require so, it is applied in a stepwise manner.

PathFinder® calculates the entire grade slate optimization on a Pentium II 450MHz platform in less than 8 hours, with a mean of 5 nonlinear model evaluations to find the optimal trajectory. The same grade slate was optimized with an SQP method, where all the model evaluations are performed on the nonlinear model, resulting in 140 hours of computation time. In Fig. 6 a representative comparison between SQP and SSQP (with regard to number of nonlinear model evaluations) is shown.

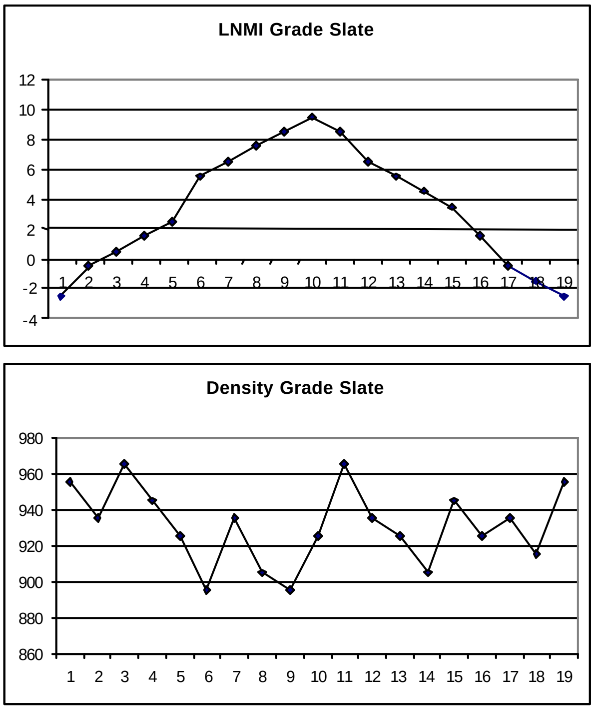


Fig. 5 Benchmark HDPE Grade Slate

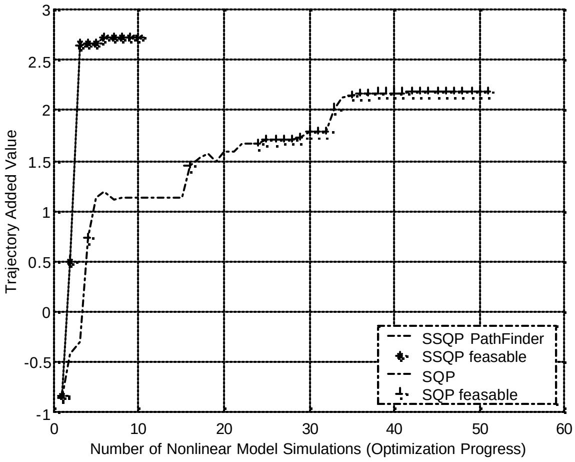
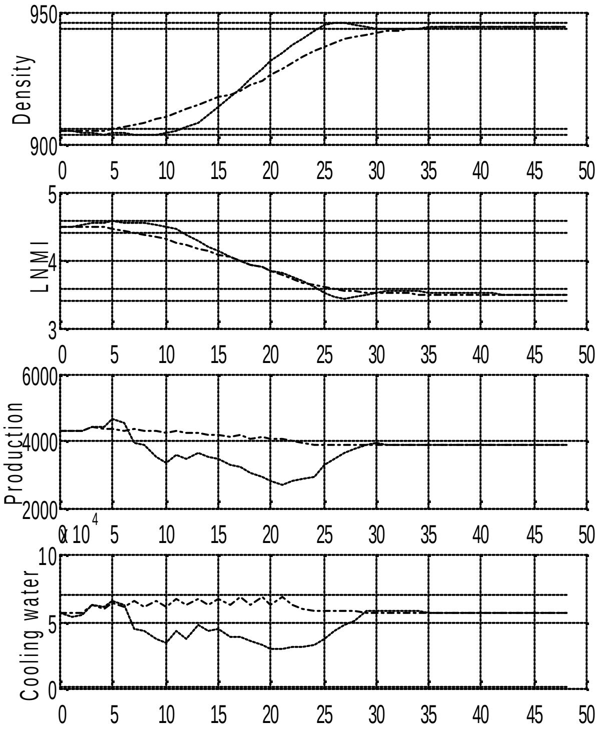


Fig. 6 Comparison between an SSQP optimizer and an SQP optimizer.

In Fig. 7 some process values of an optimized trajectory are shown. The lines indicate the ranges of the respective grades and the cooling water constraint. In Fig. 8 the manipulated variables (the optimization parameters) are shown. The move times can easily by distinguished.



change. The dashed lines represent the initial trajectory, while the solid lines correspond to the optimized trajectory.

The price of the starting grade is 0.67 €/kg, while the end grade is worth 0.73 €/kg. The off-spec material is only worth –0.1 €/kg, which is less than the operation cost at that moment. This makes it very important to minimize the production of off-spec material.

The optimized grade change discussed above results in an extra added value (compared with the typical case) of 52.000 €/changeover compared to the steady state transition.

Two important results from the dynamic optimizer can be distinguished:

1. The optimized grade change occurs considerably faster than a traditional grade change. The melt index was only 12 hours off-spec compared to 25 hours in the steady state situation. In fact, both density and melt index show undershoot and overshoot behavior although these phenomena stay within the allowable grade-range. These dynamic effects realize maximum

benefits during the grade transition. The MV's also show the dynamic actions

2. Notice how the productivity is reduced during the grade-change. At that time the operation costs are larger than the revenues, urging for reduced production

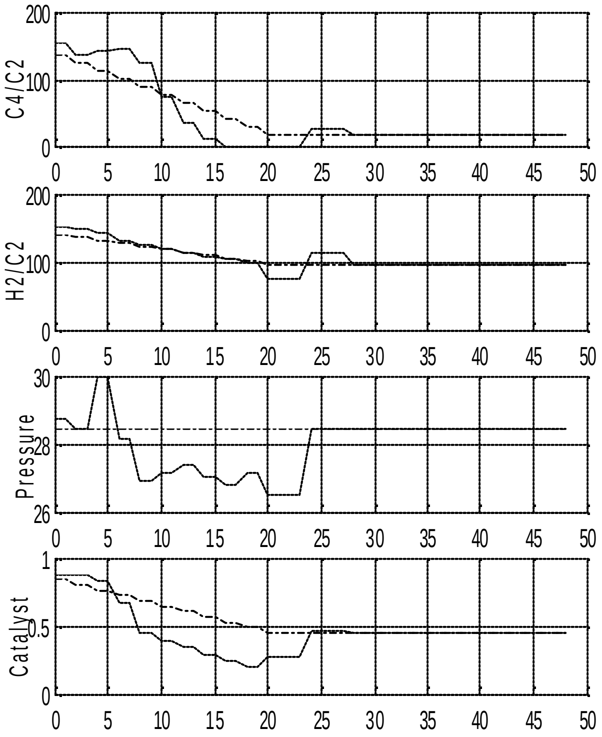


Fig. 8 Manipulated Values for an optimized grade change. The dashed lines represent the initial trajectory, while the solid lines correspond to the optimized trajectory.

5. CONCLUSION

A robust optimization technology Pathfinder® for the calculation of economical optimal grade change trajectories has been presented. Key requirements of the new technology are calculation speed due to the high non-linearity of the economic objective function and the long calculation time of rigorous model simulations. The application of an SSQP and a modified Trust Region approach proves to be an adequate solution for this problem.

Pathfinder® has been extensively and successfully tested on a rigorous model of an HDPE Fluidized Bed Gasphase reactor. In general it proved to be nearly 20 times faster than a traditional SQP optimization approach, which makes a practical application feasible. A considerable economic benefit can be obtained optimizing dynamically the transition trajectory as well as the product throughput at that time.

6. ACKNOWLEDGEMENTS

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