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# A high performance model predictive controller: application on a polyethylene gas phase reactor

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**Abstract**

This paper describes the development of a new model predictive control technology INCA® that enables a high performance demand driven operation in the chemical process industry. The technology sustains optimal grade changes, maintains tight quality control and leads to low application development and implementation costs. An application on a polyethylene gasphase reactor is discussed. 

*Keywords:* Predictive control; Model based control; Optimal trajectory; 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 optimal control of grade transitions such that these transitions become feasible and economically attractive. Also tight quality control is needed, requiring large bandwidth controllers and inferential sensors. Finally the application cost and the implementation cost must be reduced to make these projects economically attractive. This is done by using as much a-priori knowledge as possible.

INCA® has been developed for these purposes (Ludlage & Backx, 1999). An application on a polyethylene gasphase reactor is discussed.

The idea of optimization of grade transitions has been introduced by McAuley (McAuley & 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, Tousain, Backx, & Bosgra, 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.

Control of grade transitions has been studied by several authors. Lines (Lines et al., 1993) addresses the problem by formulating a NLMPC problem. The original non-linear problem is replaced by a time variant linear problem where models are subject to gain scheduling.

Wang (Wang et al., 2000) integrates the controller with an off-line optimized trajectory. A NLMPC problem is stated using a non-linear model with its linearized version.

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In this paper a new method is presented to integrate off-line trajectory optimization with feedback control. The so-called delta-mode controller compensates for deviations from a given input–output trajectory on both the process inputs and outputs.

The paper is organized along the following three Sections:

- In Section 2 the economic background showing the needs for a new process operation is explained. This process operation requires high performance process control technology.
- Subsequently, in Section 3 the requirements for the new process control technology are discussed. An answer to all these technological challenges, INCA®, is presented.
- Finally, Section 4 describes the application of INCA® 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 predominantly moving towards *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, Bosgra, & Marquardt, 1998). 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.

However, a demand driven operation of production processes requires a *new technology* that enables:

- *Flexible operation* of plants over broad operating ranges at minimum costs. In fact, a technology is needed that supports transitions between grades, such that these transitions become feasible and are economically justified. Dynamic optimization is needed to realize overall optimization of economic performance, leading to optimal grade changes.
- *Tight production* at pre-specified $C_{p_k}$ (capability) values (Eq. 2), requiring high performance model based control systems that enable significant reduction of variance of critical process/product variables.
- Extensive use of available a-priori knowledge, such as models used for design purposes, to minimize *total application costs* and to enable economic feasibility.

Each of these key requirements will be treated in more detail in Section 3.

## 3. INCA®: a new technology

A new technology INCA® is developed that makes flexible operation combined with tight production at a reasonable application cost feasible.

INCA® is a complete family of on-line and off-line components specifically designed to support the industrial application and implementation of control. The engine of INCA® is a generally applicable supervisory model predictive controller that meets current operating requirements for a broad variety of different process industries, e.g. glass industry, chemical and polymer industry.

It therefore incorporates the basic functionality that can be found in industrial model predictive controllers. The control problem is solved basically in three steps:

- Prediction of the future behavior of the process based on assumed future behavior of the process inputs.
- Minimization of the difference between predicted future steady state process behavior and the desired behavior of the process. The minimization problem is formulated as a ranked constrained quadratic optimization problem: ranked classes are used to give a class of requirements absolute priority above lower ranked classes and at the same time the solution for current class by the solution of the higher ranked classes. Requirements can be both setpoints and constraints. In one class violation of constraint limits and deviation from setpoints are traded-off based on a constrained weighted quadratic optimization. The solution for this class is then added to the set of constraints used to solve the lower ranked classes. The ranked specification approach enables the control engineer to specify a control strategy that closely resembles the actual operational hierarchy of the plant or unit.

- In the last step a constrained quadratic optimization problem is solved that brings the process from the current process conditions to the calculated steady state conditions. As in (Muske & Rawlings, 1993) this problem is formulated as a regulator problem.

Besides the functionality described before, extra functionality is added to improve the model predictive controller in order to improve production flexibility, to achieve tight quality control and to reduce total application costs.

The *production flexibility* is enhanced by the use of a rigorous non-linear dynamic model. Models are typically widely available in chemical industry since they are used for design purposes. Specific extensions to these models make them suited for dynamic optimization purposes oriented towards optimal trajectory calculation. These optimal trajectories not only provide economically optimal grade transitions and thus production flexibility, but also guarantee continuous optimal disturbance recovery in normal operation.

The dynamic optimizer tries to maximize added value (AV) (Van der Schot et al., 1999). The added value depends on the throughput. It is a non-linear function with regard to operation cost and a highly non-linear function with regard to product price as indicated before (cf. Eq. 1).

$$AV(T) = \int_0^T price(t) throughput(t)\,\mathrm{d}t - \int_0^T \sum_i feed_i(t) cost_i(t)\,\mathrm{d}t + holdup(T) price(T) - holdup(0) price(0). \quad (1)$$

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 min to several hours for one simulation run.
- The highly non-linear objective function (due to the discontinuous price function for the end product being on- or off-spec) 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 standard optimization schemes. This results into a reduction of model evaluations with a factor 40, with an average of 10 rigorous model evaluations needed to obtain the optimum path. More details will be presented in a different paper.

To integrate the overall dynamic optimizer with the underlying model predictive controller, an architecture as shown in Fig. 1 is implemented. Actually the model predictive controller is operated in a delta-mode, only

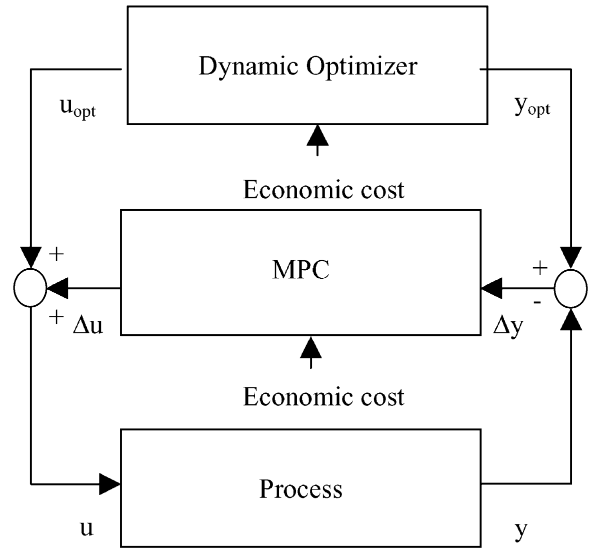


Fig. 1. Integration of the overlying dynamic optimizer with the model predictive controller.

correcting for the deviations $\Delta u$ and $\Delta y$ from the process input–output setpoints $u_{\text{opt}}$ and $y_{\text{opt}}$ that are calculated by the overall dynamic optimizer.

The delta-mode guarantees a best of both worlds operation. The trajectory has been carefully designed based on a rigorous non-linear model. 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 ($u_{\text{opt}}, y_{\text{opt}}$) 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.

Since the delta mode controller only considers deviations from a given trajectory, linear models are well suited to be used in this framework. This allows us to use a linear MPC controller with all the advantages with regard to model identification, robustness etc.

In order to avoid conflicts between the dynamic optimizer and the linear model predictive controller an economically consistent cost function for both layers is chosen.

The model predictive controller is designed such that it can make use of different linear models according to the current operation point. As such trajectories can be optimally followed. No longer one single, linear dynamic model must be used, but instead adequately tuned sets of linear models can be applied for all the different grades. During transients, the model predictive controller will smoothly switch between the different models of a set of models through a linear interpolation scheme. State estimation techniques are used to obtain a good initial estimation for the models that will be used.

A large bandwidth controller realizes *tight production at a specific $C_{p_k}$ value*. The $C_{p_k}$ value is a normalized number giving an indication about the variance $\sigma$ of a relevant process quality parameter compared to distance to the tolerance boundaries ($tol_+$, $tol_-$) (Eq. 2) (Fig. 2).

$$C_{p_k} = \frac{\min(|tol_- - Y_{mean}|, |tol_+ - Y_{mean}|)}{3\sigma}. \quad (2)$$

A large $C_{p_k}$ value corresponds to a small variance and thus a successful process operation. A $C_{p_k}$-value of 1.6 is standard, although sometimes 1.67 is already used in some cases.

The economic impact of a smaller quality variance can be understood from the shift in operation point that can be realized. In fact, a large variance forces operation to be better than desired since outliers may not exceed the tolerance boundaries. If variance is reduced, one can shift the mean operation towards the most economic boundaries, resulting in a cost reduction. This is indicated in Fig. 2.

A reduction in variance can only be realized by a larger bandwidth of the controller, in accordance with Parceval's theorem. This large bandwidth controller is made possible by the use of large bandwidth prediction models opposite to the traditionally applied step response models with restricted complexity. Systems with both slow and fast dynamics cannot adequately be represented by a step response model due to the fact that only a limited number of samples is available for storing the model and due to the fact that the steady state must be captured for stability reasons (Fig. 3). Therefore the fast dynamics cannot be captured in the model and reduction of the bandwidth of the controller is needed as a consequence. INCA® uses state-space models that enable the modeling of process behavior at all relevant frequencies up to the Nyquist frequency.

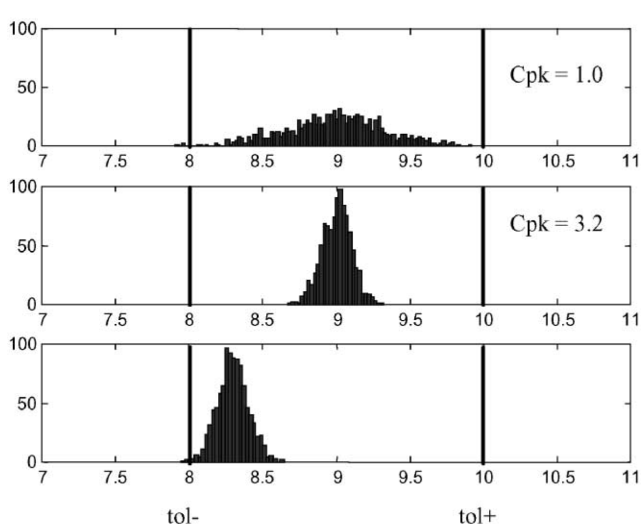


Fig. 2. Histogram of quality parameter in 3 different cases. Original situation with $C_{p_k} = 1.0$ (upper figure), reduced variance case with $C_{p_k} = 3.2$ (middle figure) and reduced variance with shift in operating point and $C_{p_k} = 1.67$ (lower figure).

Controller bandwidth can also be improved by increasing the computation speed of the MPC control algorithm. Special attention is made to the implementation of fast adapted QP/IP methodologies for this application. This also allows making use of constraints in the dynamic optimization routine.

Dynamic inferential sensors are developed for the instant calculation of product properties such as melt index, density, concentration… based on on-line process measurements. This speeds up the feedback loop since lab analysis results must no longer be waited for, thus leading to further improvement in the closed loop controller bandwidth.

A *reduction of the total application cost* is obtained by making maximum use of a priori knowledge. In fact, the dynamic model applied in the controller can be understood as a combination of a first principles based model part, describing the main process mechanisms, and an empirical model part describing specific dynamic process characteristics that cannot be modeled sufficiently accurately for control on the basis of first principles. The first part mainly describes physical phenomena. Chemical phenomena often require empirical modeling due to unknown or only roughly known reaction complexes and reaction kinetics.

The first principle part can be tuned based on the design data and historical data of the plant under concern. A dominant part of these dynamics corresponds to the physical phenomena, which are predominantly low frequent and which can be modeled accurately on the basis of first principles. Once a plant model template has been realized, this model is tuned by optimization techniques such as simulated annealing.

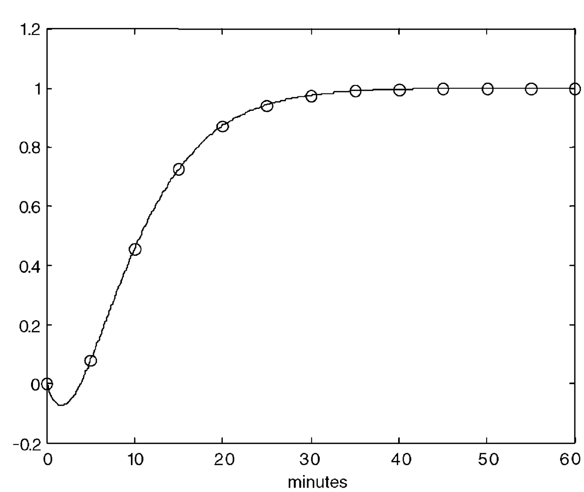


Fig. 3. A step response (here shown with 12 samples for illustrative purposes) cannot capture high-frequent behavior such as a fast non-minimum phase response.

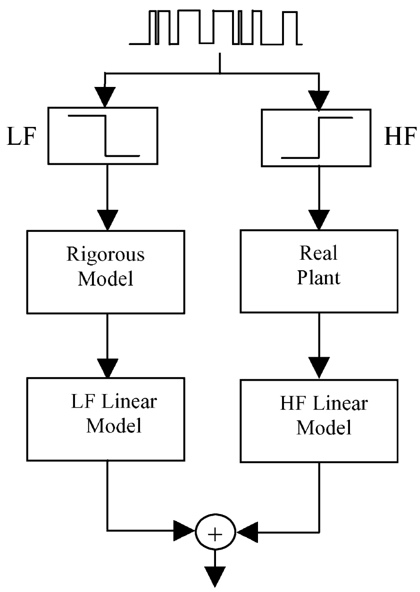


Fig. 4. Combination of low frequency identification on the rigorous model and high frequency identification on the plant.

The chemical parts of the model and the properties will be a mixture of first principle parts and empirical parts. Some well-defined experiments are needed to tune these parts of the model. These experiments do not take much time, since the related phenomena are considerably faster than the previously mentioned physical phenomena related to mass and energy balancing, transport phenomena etceteras.

Concerning the linear models needed for the model predictive controller, the model identification is done in parallel on the plant for the high frequencies and on the rigorous model for the slow dynamics, as shown in Fig. 4 (cf. (Backx, 1999)).

Since only high frequency components have to be estimated on the real plant, short dedicated PRBNS tests are sufficient, in contrast to the long experiments that are needed for the identification of step response models. This results in a significant reduction of project engineering hours and thus application development costs.

A second means of reducing the application cost is to re-use the knowledge in several applications. As such special shells are being developed for the polyethylene, polypropylene and PET industry.

## 4. Application: the polyethylene gasphase reactor

The INCA® technology mentioned before is applied to a HDPE fluidized bed gas phase reactor. A complete rigorous dynamic model for the polyethylene gas phase reactor has been developed in *gPROMS* based on the model that was proposed by Choi and Ray (Choi & Ray, 1992) and the Ph.D. thesis of McAuley (McAuley, 1991).

The process is depicted in Fig. 5. 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. 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.

The entire process to be controlled by a supervisory model predictive controller shows 4 manipulated variables (mv) and 4 controlled variables (cv), as indicated in Fig. 5. The purge valve is not used as a manipulated variable in order to avoid economic losses.

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

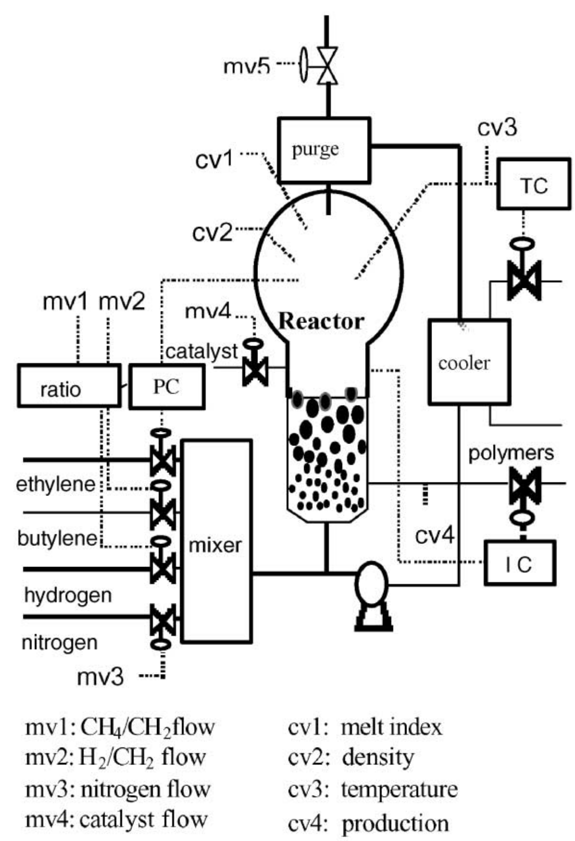


Fig. 5. Polyethylene Gasphase Reactor Process.

In Fig. 6 the most important process variables of a typical grade change and an optimal grade change supported by INCA® are shown, while the manipulated variables are given in Fig. 7. An operator, who takes some manipulated variables on manual, typically performs the grade change. This 'manual' grade change is given in dashed lines.

The lines in the Density and LNMI graph (Fig. 6) indicate the specification ranges of the respective grades. The price of grade A is 0.67 €/kg, while grade B is worth 0.73 €/kg. The off-spec material is only worth 0.57 €/kg, which is less than the operation cost at that moment. This makes it very important to minimize the production of off-spec material. To maximize added value over the time interval covering the full grade change an optimum has to be searched that trades off the amount of off-spec material produced against lost production time due to reduction of productivity during the grade change. The transition needs to be done such a way that the added value is continuously maximized within the feasible operating region. The operating region is e.g. restricted by the available cooling water flow, as indicated by the straight line in the lower graph of Fig. 6.

The underlying INCA® model predictive controller supports such a non-linear excursion from one grade to another as discussed before. In fact it is almost transparent in the results presented here.

Two important results from the dynamic optimizer can be distinguished:

1. The MPC controlled grade change occurs considerably faster than a traditional grade change. The melt index was only 12 h off-spec compared to 25 h in the normal situation. In fact, both density and melt index show undershoot and overshoot behavior, although these phenomena stay within the allowable grade specification range. These dynamic effects realize maximum benefits during the grade transition. Note that a high performance MPC is needed to track these trajectories. It is also needed to switch between different linear models, since this is a large transition between different grades. In this case two linear models are being used. Neural-net based soft-sensors are implemented to track quality parameters such as density and melt-index on-line.
2. In Fig. 6 the productivity is shown. 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.

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

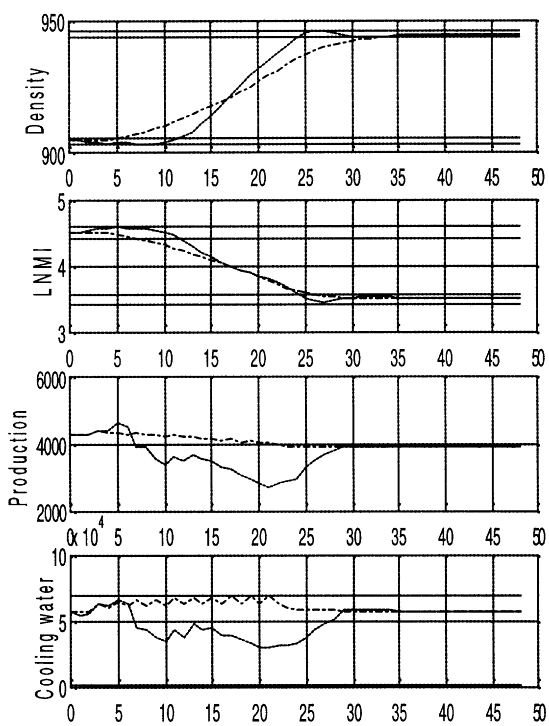


Fig. 6. Process values for an optimized grade change. The dashed lines represent the initial trajectory, while the solid lines correspond to the optimized and controlled trajectory.

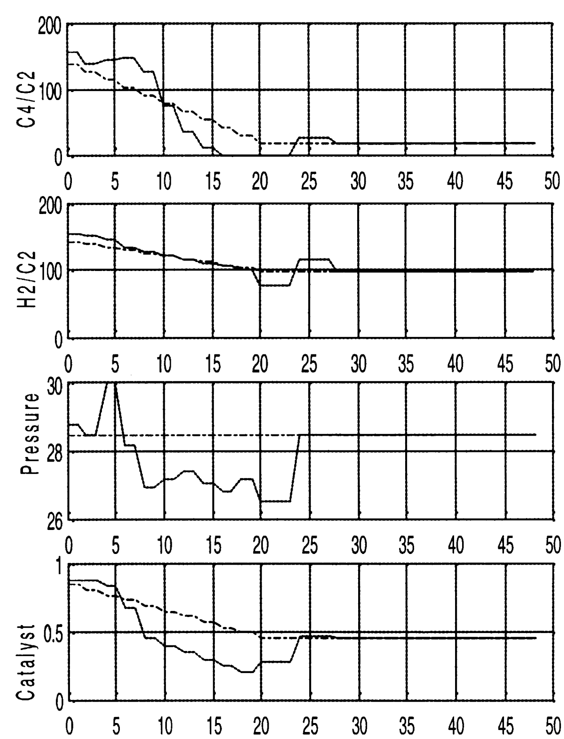


Fig. 7. Manipulated values for an optimized grade change. The dashed lines represent the initial trajectory, while the solid lines correspond to the optimized and controlled trajectory.

## 5. Conclusion

An advanced model predictive control technology based on rigorous dynamic models has been presented. Key requirements of the new technology are the realization of a flexible process operation, a large bandwidth control enabling tight quality control and low application costs. The flexible operation is realized by the combination of a dynamic optimizer over a rigorous model together with a model predictive controller in delta-mode. A large bandwidth control is enabled by the use of high frequent prediction models. Ultimately, re-use of large parts of rigorous models for different applications together with low frequency testing on these rigorous models reduces the application cost.

The application of the before mentioned technology is shown successfully on a polyethylene gasphase reactor simulator. A considerable economic benefit can be obtained optimizing the transition trajectory as well as the throughput at that time.

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