99-58

ADCHEM 2000

INTERNATIONAL SYMPOSIUM ON ADVANCED CONTROL OF CHEMICAL PROCESSES

Pisa, Italy, June 14-16, 2000

PREPRINTS

VOL. I

Pages 1 - 676

Papers of the 1st and 2nd day

EDITORS

Lorenz T. Biegler
Carnegie Mellon University, Pittsburgh PA - USA
Alessandro Brambilla
University of Pisa, Pisa - Italy
Claudio Scali
University of Pisa, Pisa - Italy

ASSISTANT EDITOR

Gabriele Marchetti
University of Pisa, Pisa - Italy

ADCHEM 2000
INTERNATIONAL SYMPOSIUM ON ADVANCED CONTROL OF CHEMICAL PROCESSES
Pisa, Italy - June 14-16, 2000

IFAC

A HIGH PERFORMANCE MODEL PREDICTIVE CONTROLLER: APPLICATION ON A POLYETHYLENE GAS PHASE REACTOR

Wim Van Brempt, Ton Backx, Jobert Ludlage, Peter Van Overschee, Bart De Moor, R. Tousain

Wim Van Brempt, Peter Van Overschee
ISMC NV. Kardinaal Mercierlaan 94, 3001 Heverlee, Belgium
Wim.VanBrempt@ismc.be Peter.VanOverschee@ismc.be

Ton Backx, Jobert Ludlage
IPCOS Technology b.v. Bosscheweg 145a, 5282 WV Boxtel, The Netherlands
Ton.Backx@ipcos.nl, Jobert.Ludlage@ipcos.nl

Bart De Moor
ESAT-SISTA, K.U. Leuven, Kardinaal Mercierlaan 94, 3001 Heverlee, Belgium
bart.demoor@esat.kuleuven.ac.be

Rob Tousain
Mechanical Engineering Systems and Control Group
Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands
R.L.Tousain@WBMT.TUDELFT.NL

*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 et al, 1999]. An application on a polyethylene gasphase reactor is discussed.

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 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]. 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 Cp_k values, 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.

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.

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 correcting for the deviations Δu and Δy from the process input-output setpoints u_{opt} and y_{opt} that are calculated by the overall dynamic optimizer. This delta-mode guarantees that an optimal operation as calculated by the optimizer, is not cancelled by the underlying model predictive controller.
In order to avoid conflicts between the dynamic optimizer and the model predictive controller an economically consistent cost function for both layers is chosen.

The model predictive controller is also 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.

A large bandwidth controller realizes **tight production at a specific Cp_k value.** The Cp_k value is a normalized number giving an indication about the variance σ of a relevant process quality parameter compared to distance to the tolerance boundaries (tol_+, toL) (Eq. 1) (Fig. 2).

$$Cp_k = \frac{\min(|tol_- - Ymean|, |tol_+ - Ymean|)}{3\sigma} \quad (1)$$

A large Cp_k value corresponds to a small variance and thus a successful process operation. A Cp_k-value of 1.3 is standard, although sometimes 1.6 is already used in some cases.

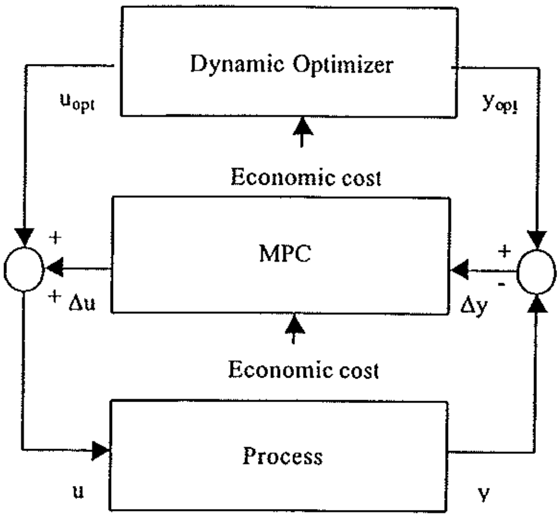


Fig. 1. Integration of the overlying dynamic optimizer with the model predictive controller

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.

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 no longer must be waited for lab analysis results, thus leading to further improvement in the closed loop controller bandwidth.

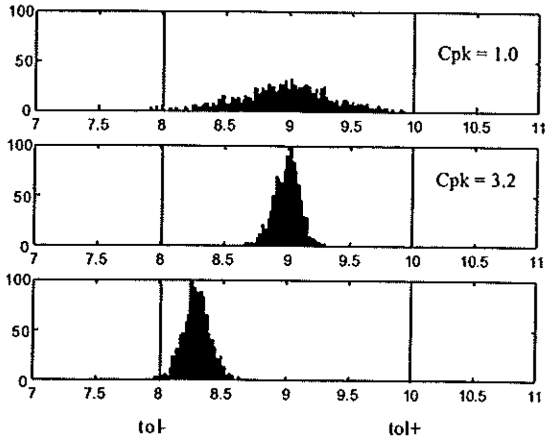


Fig. 2. Histogram of quality parameter in 3 different cases. Original situation with Cp_k = 1.0 (upper figure), reduced variance case with Cp_k = 3.2 (middle figure) and reduced variance with shift in operating point and Cp_k = 1.0 (lower figure)

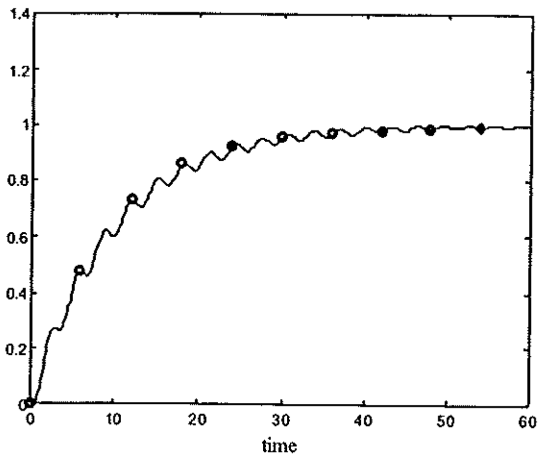


Fig. 3 A step response (here shown with 10 samples for illustrative purposes) cannot capture high-frequent behavior

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.

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 etcetera.

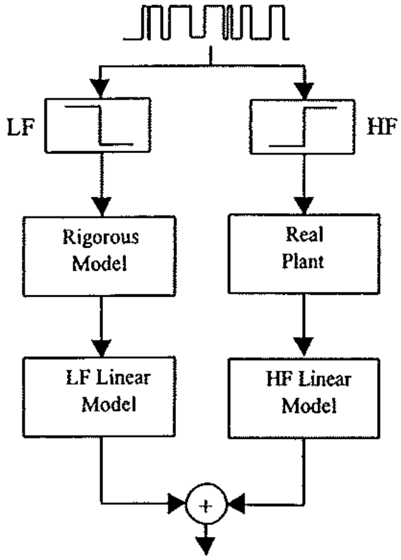


Fig. 4 Combination of low frequency identification on the rigorous model and high frequency identification on the plant.

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 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*.

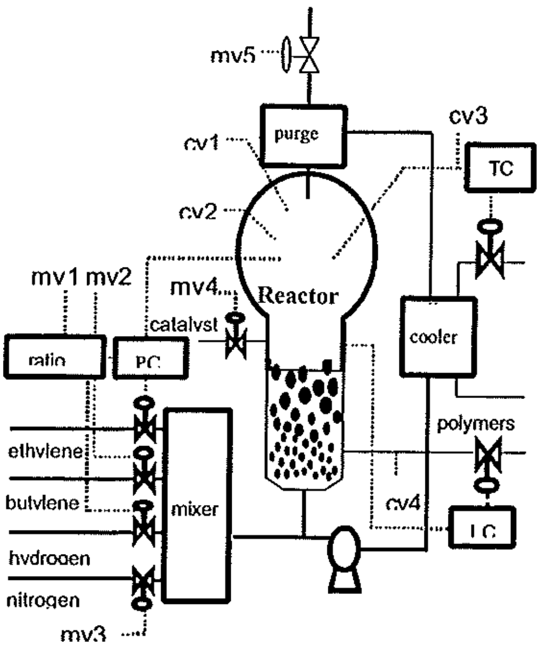
The process is depicted in Fig. 5. The ethylene monomer and butylene co-monomer react to HDPE. The unreacted ethylene goes to the top of the reactor and is recycled. The butylene/ethylene (CH_4/CH_2) ratio and the hydrogen/ethylene (H_2/CH_2) ratio are crucial handles to obtain HDPE with the desired 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

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.

In Fig. 6 and Fig. 7 a typical grade change is shown. An operator, who takes some manipulated variables on manual, typically performs the grade change. The other variables are controlled by PID-controllers.

The bold-face lines indicate the 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.



mv1: CH_4/CH_2 flow
mv2: H_2/CH_2 flow
mv3: nitrogen flow
mv4: catalyst flow

cv1: melt index
cv2: density
cv3: temperature
cv4: production

Fig. 5 Polyethylene Gasphase Reactor Process

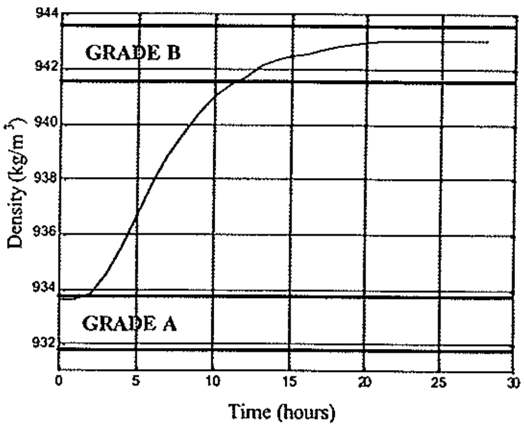


Fig. 6. A typical HDPE Density Grade Change.

In Fig. 8 and Fig. 9 an optimized grade change supported by INCA® and the overall optimizer is shown.

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 nonlinear function with regard to operation cost and a highly non-linear function with regard to product price as indicated before (cf. Eq. 2).

$$AV(T) = \int_0^T price(t) throughput(t) dt - \int_0^T \cos t(t) dt + holdup(T) price(T) - holdup(0) price(0) \quad (2)$$

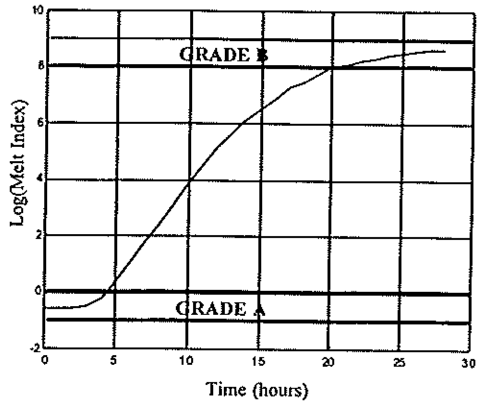


Fig. 7. A typical HDPE Melt Index Grade Change

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 11 hours off-spec compared to 16 hours in the normal 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. 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. Soft-sensors are implemented to track quality parameters such as density and melt-index on-line.

2. In Fig. 10 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 8.500 €/changeover (compare 11.000€ for Fig. 6 and Fig. 7 to 19.500€ for Fig. 8 and Fig. 9).

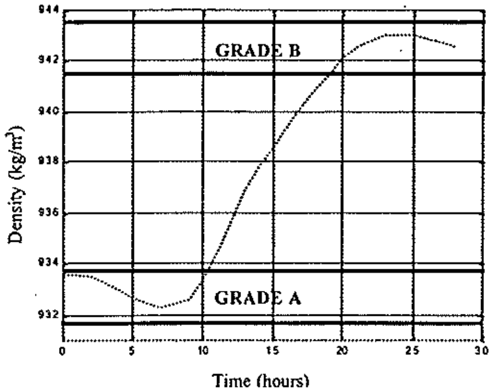


Fig. 8 HDPE Density Grade Change using the INCA® model predictive controller in delta-mode in combination with the dynamic optimizer.

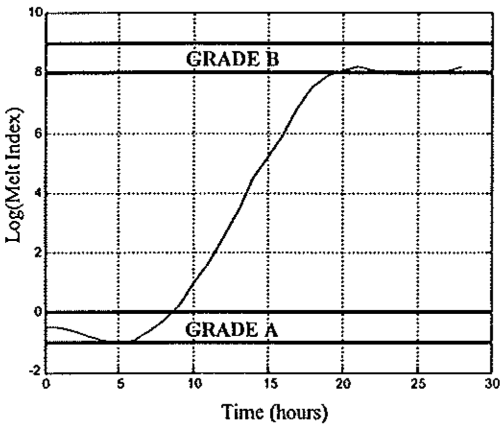


Fig. 9. HDPE Melt Index Grade Change using the INCA® model predictive controller in delta-mode in combination with the dynamic optimizer.

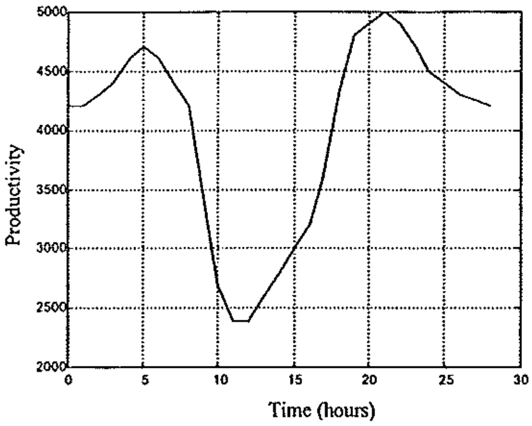


Fig. 10. Reactor Productivity during grade change using the INCA® model predictive controller in delta-mode in combination with the dynamic optimizer.

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.

6. ACKNOWLEDGEMENTS

This work is supported by the IWT (Flemish Institute for Science and Technology in Industry) project IMPACT (EUREKA 2063): Improved Polymer Advanced Control Technology. The scientific responsibility is assumed by its authors.

REFERENCES

Backx, T., O. Bosgra and W. Marquardt, 1998, Towards intentional dynamics in supply chain conscious process operations, proc. FOCAPO 1998, 5-7 July 1998, Snowbird Resort, Utah, USA

Backx, T., 1999, Combining first principles dynamic modelling and plant identification for design of an industrial MPC application top a polymer reactor, Preprints IFAC 14-th World Congress, 5-9 July 1999, Beijing, P.R.China, Vol. N, pp 61-66

Ludlage, J. and T. Backx, 1999 A new generation model predictive control technology, proc. 5-th international seminar on mathematical simulation in glass melting, June 17-18, 1999, Horni Becva, Czech Republic, pp 170-180

Van der Schot, J.J., R.L. Tousain, A.C.P.M. Backx and O.H. Bosgra, 1999, SSQP for the solution of large scale dynamic-economic optimization problems, proc. ESCAPE 1999, June 1999, Budapest, Hungary