

# Simultaneous Data Reconciliation and Parameter Estimation in Bulk Polypropylene Polymerizations in Real Time

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**Summary:** This work presents the implementation of a methodology for dynamic data reconciliation and simultaneous estimation of quality and productivity parameters in real time, using data from an industrial bulk Ziegler-Natta propylene polymerization process. A phenomenological model of the real process, based on mass and energy balances, was developed and implemented for interpretation of actual plant data. The resulting nonlinear dynamic optimization problem was solved using a sequential approach on a time window specifically tuned for the studied process. Despite the essentially isothermal operation conditions, obtained results show that inclusion of energy balance constraints allows for increase of information redundancy and, as a consequence, for computation of better parameter estimates than the ones obtained when the energy balance constraints are not considered (Prata *et al.*, 2005). Examples indicate that the proposed technique can be used very effectively for monitoring of polymer quality and identification of process malfunctions in real time even when laboratory analyses are scarce.

**Keywords:** modeling; nonlinear dynamic data reconciliation; on-line process monitoring; parameter estimation; Ziegler-Natta polymerization

## Introduction

Process measurements are normally taken for implementation of process control procedures and evaluation of process performance. With the advent of modern desktop computers, hundreds or thousands of process measurements are simultaneously measured and stored in massive storage media for the continuous monitoring of the process behavior and for performing process studies, such as the development of robust process models and the online optimization of the process operation. Therefore, modern industrial plants may provide very detailed and rich data sets for development of fundamental modeling studies. However,

as a result of random and possibly gross errors (caused by instrument failure and/or instrument miscalibration) process measurements do not generally satisfy process constraints (such as mass and energy balances). Thus they need to be reconciled.

Data reconciliation may be defined as the adjustment of process measurements and parameters in order to satisfy a certain set of constraints while minimizing some sort of objective function that weighs the deviations observed between corrected and observed plant values. The estimation of process model parameters from available plant data is certainly in this context. First, the mathematical model provides the process constraints to be satisfied. Second, model parameters (and process measurements) have to be adjusted to minimize the deviations observed between process measurements and process constraints. For this reason, available data have to be filtered to

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allow for removal of inconsistent data sets from the process data used for model building.

In chemical engineering, for steady-state process, Kuehn and Davidson (1961)<sup>[1]</sup> presented the seminal paper describing the data reconciliation problem, presenting the general solution when all flows are measured. The literature regarding data reconciliation strategies is huge and good reviews can be found in the literature.<sup>[2–5]</sup>

Important data reconciliation applications involve the so-called gross error detection schemes.<sup>[6]</sup> These techniques combine parameter estimation procedures and statistical inferential criteria to allow for identification of outliers among available process data. Gross error detection is of fundamental importance for adequate model building and interpretation, as poor input data generally lead to very poor model responses. The simplest gross error detection tests compare nominal measurement errors with observed model deviations, assuming the normal distribution of measurement errors around zero, and remove (or correct) data points that do not follow the normal assumption. Although usual, the normality of the error distribution is not needed for gross error detection.<sup>[7]</sup>

Alternative approaches to gross error detection involve the use of principal component analysis,<sup>[8]</sup> cluster analysis,<sup>[9]</sup> artificial neural networks<sup>[10]</sup> or robust statistics.<sup>[11]</sup>

Traditional data reconciliation techniques assume that the process is at steady-state conditions and that process constraints are linear.<sup>[3]</sup> Thus, for these techniques to be applied it is necessary to guarantee that process data are obtained at steady-state conditions.<sup>[12]</sup> None of these two assumptions are actually necessary for data reconciliation to be carried out, as the nonlinear,<sup>[13]</sup> dynamic<sup>[14]</sup> and both nonlinear/dynamic<sup>[15,16]</sup> nature of the model constraints may be preserved. In these cases, the reconciliation data problem is formulated as a traditional parameter estimation problem and is solved through

standard numerical procedures, such as sequential quadratic procedures<sup>[17]</sup> and quasi-Newton algorithms.<sup>[18]</sup>

As the data reconciliation problem may be formulated as a traditional parameter estimation procedure, it is not surprising to observe that some authors suggest that both process states and parameters be estimated simultaneously.<sup>[15,19]</sup> This way, important parameters that are difficult to measure on-line (such as kinetic constants and heat transfer coefficients) are obtained during the data reconciliation process. This procedure also allows for more detailed fundamental models, which depend on unknown parameters, to be used as model constraints during data reconciliation.

### Data Reconciliation in Polymerization Systems

Although data reconciliation procedures are intended to be used at plant site, very little is described in the open literature about the use of data reconciliation procedures in actual industrial applications. Besides, the simultaneous reconciliation of data sets and estimation of model parameters using dynamic models has not been widely reported,<sup>[20]</sup> especially with real polymerization processes and plant data.

It seems that the first study regarding the estimation of model parameters and application of data reconciliation procedures for polymerization systems is presented by Sirohi and Choi (1996).<sup>[21]</sup> In this paper, the control of an olefin gas-phase fluidized bed reactor is studied, based on a simple process model. A numerical strategy based on the extended Kalman filter and on a nonlinear recursive estimation algorithm was devised to allow for the online estimation of three key kinetic parameters and for improvement of the controller performance during catalyst exchange operation. The kinetic parameters were adjusted to fit the catalyst activity, the polymer composition and the weight average molecular weight of the final polymer material. The application was based on simulated data and the

performance of the algorithm in actual industrial examples was not shown.

Barbosa Jr. *et al.* (2000)<sup>[22]</sup> applied the simultaneous solution approach, originally developed by Liebman *et al.* (1992),<sup>[16]</sup> to solve the problem of nonlinear dynamic data reconciliation of free-radical bulk styrene polymerizations performed in CSTRs. Only simulated data were analyzed.

Kiparissides *et al.* (2002)<sup>[23]</sup> performed the simultaneous state and parameter estimation in order to allow for the online optimization of industrial polymerization reactions. Actual industrial data were not presented.

Bindlish *et al.* (2003)<sup>[24]</sup> estimated two kinetic parameters using industrial data obtained from polymerization process from 13 data sets provided by Exxon. They showed the confidence interval of the estimation result, but model parameters were not allowed to vary along the process operation.

Vieira *et al.* (2003)<sup>[25]</sup> studied a polymerization process and developed a process model based on real industrial data. Most of the model parameters were obtained from available published material, but some of the unknown parameters were estimated using simultaneous data reconciliation and parameter estimation procedures. The studied system comprised a sequence of polymerization reactors, arranged in series and/or parallel, depending on the particular produced resin grade. The simultaneous nonlinear dynamic data reconciliation and parameter estimation problem was solved with a standard Gauss-Newton estimation procedure.<sup>[26]</sup> Nineteen process parameters were estimated and analyzed off-line for distinct data sets.

Arora and Biegler (2004)<sup>[20]</sup> applied the nonlinear trust-region estimator in order to estimate model parameters on line for a polymerization reactor model. Only simulated data were analyzed.

Prata *et al.* (2005)<sup>[27]</sup> applied simultaneous nonlinear dynamic data reconciliation and parameter estimation procedures in order to monitor product quality and process productivity in an industrial poly-

propylene process on-line. The studied process was the propylene bulk polymerization in a continuous stirred tank reactor and process analysis was based on real plant data. However, the model used as dynamic constraint just considered mass balances.

In this work the dynamic nonlinear data reconciliation, parameter estimation and state estimation are performed simultaneously for a real polypropylene polymerization process, using real industrial data. Model parameters and states are assumed to vary along time, in accordance with actual plant experience. The previous model described by Prata (2005)<sup>[27]</sup> and Prata *et al.* (2005)<sup>[28]</sup> is improved through incorporation of global energy balances. As shown below, this may have a tremendous effect on the overall performance of the data reconciliation scheme.

### Problem Formulation

A modified version of the estimation technique proposed by Anderson *et al.* (1978)<sup>[29]</sup> is used in this work. Measurement errors are assumed to be small, non-correlated and to occur at random. Besides, it is assumed that measurement fluctuations follow the normal distribution, with zero mean and known variance. By using the maximum likelihood principle, the associated optimization problem can be defined as:

$$\min_{\hat{\mathbf{z}}(t)} \sum_{j=0}^c [\hat{\mathbf{z}}(t_j) - \mathbf{z}_j]^T \mathbf{V}^{-1} [\hat{\mathbf{z}}(t_j) - \mathbf{z}_j] \quad (1)$$

subject to

$$\begin{aligned} \mathbf{f} \left[ \frac{d\hat{\mathbf{z}}(t)}{dt}, \hat{\mathbf{z}}(t) \right] &= 0 \\ \mathbf{h}[\hat{\mathbf{z}}(t)] &= 0 \\ \mathbf{g}[\hat{\mathbf{z}}(t)] &\geq 0 \end{aligned} \quad (2)$$

$\hat{\mathbf{z}}(t)$  represents the vector of estimated functions (reconciled measurements, parameters and non-measured variables),  $\mathbf{z}(t)$  represents the discrete measured values,  $\mathbf{V}$  is a diagonal matrix of measurement error variances,  $\mathbf{f}$  represents the dynamic constraints,  $\mathbf{h}$  and  $\mathbf{g}$  are equality and inequality algebraic constraints, respectively. Vari-

ables  $t_0$  and  $t_c$  represent the initial and current times, respectively.

Several strategies have been proposed to solve such constrained nonlinear dynamic programming problems.<sup>[30]</sup> In this work, a sequential strategy is applied to a time varying moving window. For practical implementation on dynamic systems, it is common to use a time varying moving window (moving horizon) in order to reduce the optimization problem to manageable dimensions.<sup>[5]</sup> The window size is a tuning parameter that is utilized to capture the latest process behavior,<sup>[9]</sup> being useful when process parameters can change with operational conditions.

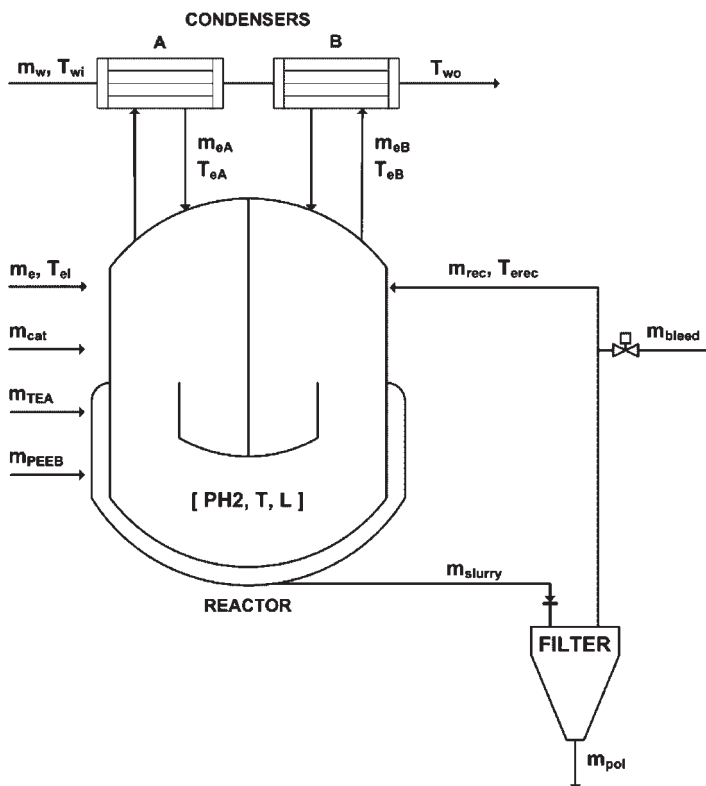
For every sample time, the differential equation system and the resulting nonlinear programming problem are solved sequentially using the data measured over the moving window, until convergence is reached. The solver used here is a standard

software for the simultaneous data reconciliation and estimation of model parameters, based on the Gauss-Newton method.<sup>[26]</sup> Convergence is controlled as proposed by Law and Bailey (1963).<sup>[31]</sup> The system of differential equations is solved numerically using DASSL.<sup>[32]</sup>

### Process Description

The analyzed process consists of the bulk polymerization of propylene in a single CSTR (LIPP-SHAC Shell Technology), with bleed and recycle streams, using high-activity fourth generation Ziegler-Natta catalyst ( $TiCl_4/MgCl_2 + PEEB + TEA$ ) to produce polypropylene in liquid propylene (liquid pool or bulk reactor).<sup>[33]</sup> This process is schematically represented in Figure 1.

Polymerization heat is removed by condensation of boiling propylene. Monomer feed rates are usually limited by maximum solid hold-up in order to keep



**Figure 1.**  
Industrial polymerization process.<sup>[33]</sup>

the suspension stable. The molecular weight distribution, estimated from the melt index (*MI*), is controlled by the hydrogen feed stream. The operation pressures are high - around 30 atm. Important issues for this technology are the control of solids hold-up, liquid propane concentration, *MI* and *XS*. The *XS* represents the fraction of polymer material that can be extracted by boiling xylene and the increase of *XS* indicates poor control of the degree of isotacticity of the polymer material. As variations of liquid propane concentration (*C<sub>a</sub>*) may prejudice polymer productivity and modify the quality of the final resin, liquid bleed flow rates (*m<sub>bleed</sub>*) must be manipulated to control the propane concentration in the liquid pool around 10%. Two important kinetic parameters can be defined in this process: *C* (kinetic constant for transfer to hydrogen, which controls the *MI*) and *K<sub>p</sub>* (kinetic constant for homo-propagation). Both constants are allowed to vary along the process operation because of modification of the levels of contaminants in the feed and because of the modifications of the hydrogen partial pressure, which is used to control the *MI* and affects the catalyst performance. The characteristic time of this process is around 1 h.

A rigorous dynamic model of this process leads to a very large system of algebraic and differential equations, which renders the on-line data reconciliation problem infeasible with current computer and numerical technology. The following simplified dynamic model has been developed to avoid this problem:

Mass Balances:

$$\frac{dPa}{dt} = m_e \cdot w_a - \left( \frac{Pa}{Pa + Pe} \right) \cdot m_{bleed} \quad (3)$$

$$\begin{aligned} \frac{dPe}{dt} = m_e \cdot (1 - w_a) - R_{pol} \\ - \left( \frac{Pe}{Pa + Pe} \right) \cdot m_{bleed} \end{aligned} \quad (4)$$

$$\frac{dPol}{dt} = R_{pol} - m_{pol} \quad (5)$$

$$\frac{dCat}{dt} = m_{Cat} - \left( \frac{Cat}{Pol} \right) \cdot m_{pol} - K_d \cdot Cat \quad (6)$$

$$\begin{aligned} \frac{dTEA}{dt} = m_{TEA} - \alpha \cdot \left( \frac{TEA}{Pe + Pa} \right) \\ \cdot m_{bleed} - (1 - \alpha) \cdot \left( \frac{TEA}{Pol} \right) \\ \cdot m_{pol} \end{aligned} \quad (7)$$

$$\frac{dPEEB}{dt} = m_{PEEB} - \left( \frac{PEEB}{Pol} \right) \cdot m_{pol} \quad (8)$$

$$\begin{aligned} \frac{d(XS)}{dt} = \frac{R_{pol}}{Pol} \\ \cdot \left[ XS^R + K_{xs} \cdot \left( \frac{TEA}{PEEB} - 1 \right) - XS \right] \end{aligned} \quad (9)$$

$$\frac{dN}{dt} = \frac{R_{pol}}{M_n^I} - \frac{m_{pol}}{M_n^{ac}} \quad (10)$$

$$m_{pol} = m_{slurry} \cdot w_{pol} \quad (11)$$

$$m_{slurry} = \frac{m_{rec} + m_{bleed}}{1 - w_{pol}} \quad (12)$$

$$w_{pol} = \frac{Pol}{M} \quad (13)$$

$$M = Pe + Pa + Pol \quad (14)$$

$$C_a = \frac{Pa}{Pa + Pe} \quad (15)$$

$$R_{pol} = \frac{K_p \cdot Cat \cdot Pe}{M} \quad (16)$$

$$MI = K_0 \cdot (M_w^{ac})^\lambda \quad (17)$$

$$M_n^I = \frac{PMPe}{\gamma + C \cdot \left( \frac{PH_2}{Pa + Pe} \right)} \quad (18)$$

$$M_n^{ac} = \frac{Pol}{N} \quad (19)$$

$$M_w^{ac} = PD \cdot M_n^{ac} \quad (20)$$

$$V = \left( \frac{Pa}{\rho_a(T)} + \frac{Pe}{\rho_e(T)} + \frac{Pol}{\rho_{pol}(T)} \right) \quad (21)$$

$$V(L) = \begin{cases} 2.300 \cdot 10^4 + [(L - 16.5\%) \cdot 1.544 \cdot 10^3] & \text{for } L > 16.5\% \\ 9.088 \cdot 10^4 \cdot [1.06 \cdot 10^{-2} \cdot L + 2.87 \cdot 10^{-4} \cdot L^2] & \text{for } L \leq 16.5\% \end{cases} \quad (22)$$

Energy Balance (EB):

$$\frac{dT}{dt} = \frac{m_e \cdot C_{pe}(T) \cdot (T_{ei} - T) + m_{rec} \cdot C_{pe}(T) \cdot (T_{erec} - T) + (-\Delta H) \cdot R_{pol} - Q_e}{(Pa \cdot C_{pa}(T) + Pe \cdot C_{pe}(T) + Pol \cdot C_{ppol}(T))} \quad (23)$$

$$Q_e = m_{eA} \cdot \lambda_e(T) + m_{eA} \cdot C_{pe}(T) \cdot (T - T_{eA}) + m_{eB} \cdot \lambda_e(T) + m_{eB} \cdot C_{pe}(T) \cdot (T - T_{eB}) \quad (24)$$

$$T_{wo} = \frac{Q_e + m_w \cdot C_{pw}(T) \cdot T_{wi}}{m_w \cdot C_{pw}(T)} \quad (25)$$

All variables are defined in the Nomenclature. The studied problem involves 15 input variables ( $m_e$ ,  $m_{cat}$ ,  $m_{TEA}$ ,  $m_{PEEB}$ ,  $m_{bleed}$ ,  $m_{rec}$ ,  $m_{eA}$ ,  $m_{eB}$ ,  $m_w$ ,  $T_{ei}$ ,  $T_{erec}$ ,  $T_{eA}$ ,  $T_{eB}$ ,  $T_{wi}$ ,  $PH_2$ ), 7 output variables ( $C_a$ ,  $m_{pol}$ ,  $XS$ ,  $MI$ ,  $L$ ,  $T$ ,  $T_{wo}$ ), 8 initial conditions for each time varying moving window ( $Pe_0$ ,  $Pa_0$ ,  $Cat_0$ ,  $TEA_0$ ,  $N_0$ ,  $XS_0$ ,  $L_0$ ,  $T_0$ ) and 2 process parameters ( $K_p$  and  $C$ ). All unmeasured variables ( $m_{slurry}$ ,  $M$ ,  $R_{pol}$ ,  $w_{pol}$ ,  $M_n^I$ ,  $M_n^{ac}$ ,  $M_w^{ac}$ ,  $Q_e$ ) can be observed with the proposed process model. Physical properties, such as densities ( $\rho_a$ ,  $\rho_e$ ,  $\rho_{pol}$ ), heat capacities ( $C_{pa}$ ,  $C_{pe}$ ,  $C_{ppol}$ ,  $C_{pw}$ ) and the heat of vaporization ( $\lambda_e$ ) are assumed to be known functions of reactor temperature. All parameter values and operational conditions are presented by Prata (2005) [27] and are not presented here for lack of space. In order to guarantee the observation of the cocatalyst concentrations, an additional algebraic equation is used as

$$PEEB_0 = \frac{(Pa_0 + Pe_0 + Pol_0) \cdot m_{PEEB}}{m_{slurry}} \quad (26)$$

### Data Analysis

The industrial data were obtained from a bulk propylene polymerization process conducted in a CSTR, as described above. During six months, six sets of actual operation data were collected to allow for

characterization of the process behavior. Each set was divided into two subsets. The first subset comprised digital data recorded automatically by the digital control system of the plant and included flow rates, temperature and pressure profiles and liquid and gas compositions provided by in-line chromatographs. The second subset comprised data recorded in process data sheets by process operators and included mostly laboratory characterization data, such as the melt index ( $MI$ ) and the xylene extractable material ( $XS$ ) of the final resin. A mathematical model was developed and implemented in order to describe the process operation, based on the detailed mass balances of the chemical components (monomer, catalyst, hydrogen, contaminants, co-catalysts, moments of the molecular weight distribution) and the global energy balance, as described previously. The final properties of the polymer resin were computed as functions of the moments of the molecular weight distribution. The magnitudes of the measurement errors (associated with the instrument) and of the process noise levels (associated with the operation) were evaluated for all process signals based on the available data at steady-state conditions. It should be noted that measured values for  $C_a$ ,  $MI$  and  $XS$  have shown small variances. The necessary redundancy for the reconciliation procedure was previously confirmed using a variable classification technique.[34]

Figures 2 to 11 present results obtained from one of the data sets, as recorded over a time interval of 7 h (29 h to 36 h), with a sample time of 5 minutes and a time window of 2 h. With a time window of 2 h (25 points – sampled 5 min/5 min), there are (15 independent + 7 dependent)  $\times 25 = 550$  variables to optimize over the window.

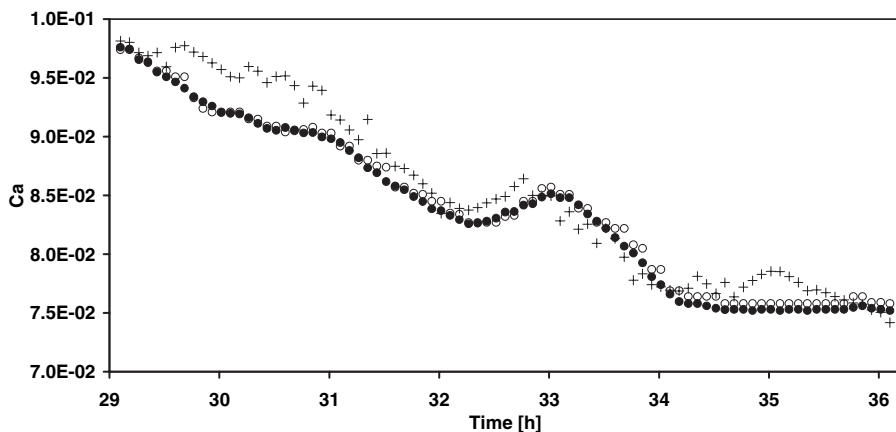


Figure 2.

$C_g$ : Measured ( $\circ$ ), reconciled ( $\bullet$ ), reconciled without EB (+).

Figures 2 and 3 show measured and reconciled data for the propane concentration in the recycle stream and for the produced polymer flowrate, respectively. For propane concentration, reconciled data with and without the energy balance (EB) are compared. It can be seen that inclusion of the energy balance leads to better results as the reconciled values are closer to the measured data, with less oscillation. Figure 3 shows that polymer production decreased along the analyzed time window. In this particular case, the mass flowrates of polymer production are subject to signifi-

cant levels of noise, because the rates of polymer production are evaluated at the storage tanks, and not at the outlet reactor stream. Therefore, the reconciled values probably represent the actual process operation conditions much more accurately than the available measured data, which incorporate production lags and other types of process fluctuations.

The decrease of polymer production is clearly detected by the  $K_p$  parameter (associated with the reaction rates), as shown in Figure 4. Similar behavior can be observed in Figure 5, which represents

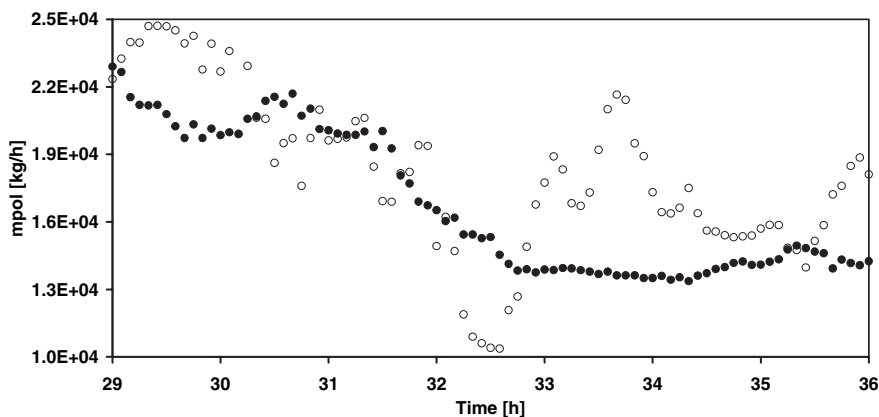


Figure 3.

$m_{pol}$ : Measured ( $\circ$ ), reconciled ( $\bullet$ ).

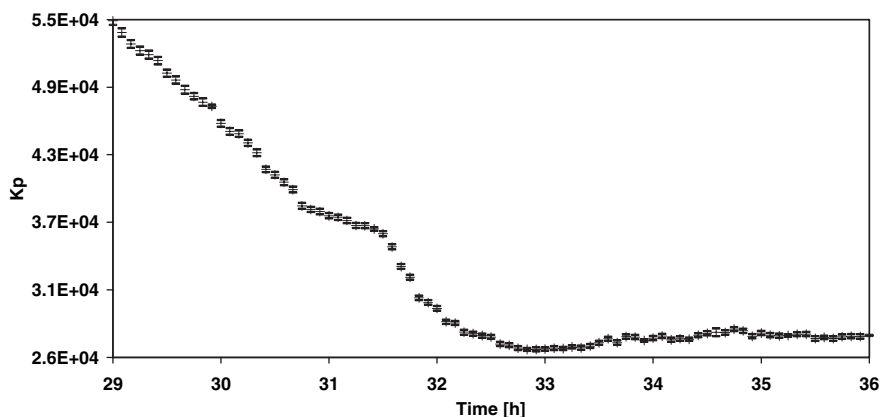


Figure 4.

$K_p$ : Estimated (+), error limits (–).

the estimation of the  $C$  parameter (associated with the  $MI$ ). It seems clear that the performance of the catalyst system is changing at the plant during the analyzed time window. One should also observe that the 95% confidence limits of the parameters  $K_p$  and  $C$  are very small and uniform. As the parameters change along the time at plant site, model parameters should not be used for prediction of future process responses without careful analysis of the process behavior and output trends.

Figures 6 and 7 show measured and reconciled data for hydrogen pressure in the reactor and for  $PEEB$  input flowrates,

respectively. In both cases very good filtering of measured data can be observed. It becomes very clear that the parameter  $K_p$  depends on the hydrogen concentration and on the  $PEEB$  input flowrate, as significant decrease of the  $K_p$  estimates can be observed after grade transition (increase of  $PH_2$  and decrease of  $m_{PEEB}$ ). This piece of information may be valuable for optimization of the process operation, as additional catalyst feed would be required to keep the polymer production constant.

Figures 8 and 9 show measured and reconciled data for temperature in the

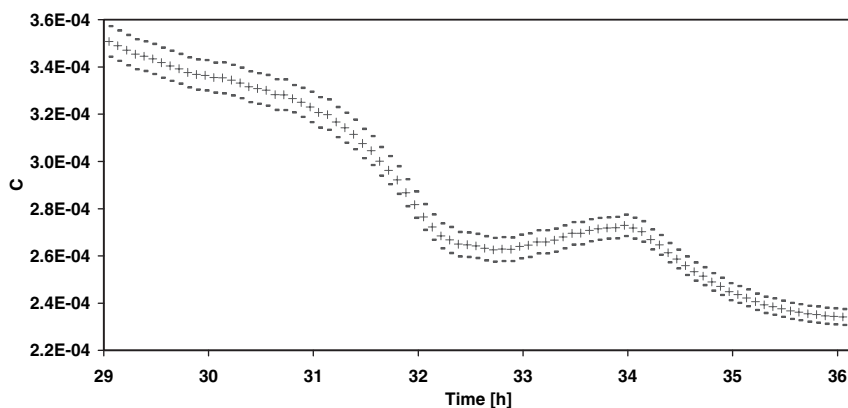


Figure 5.

$C$ : Estimated (+), error limits (–).



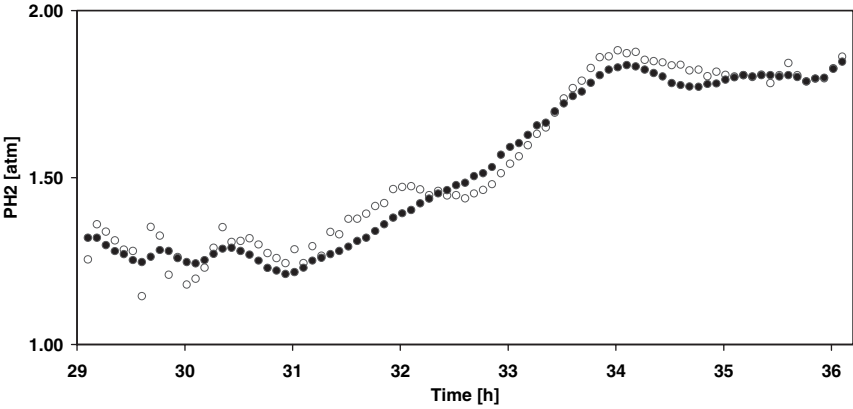


Figure 6.  
 $PH_2$ : Measured (○), reconciled (●).

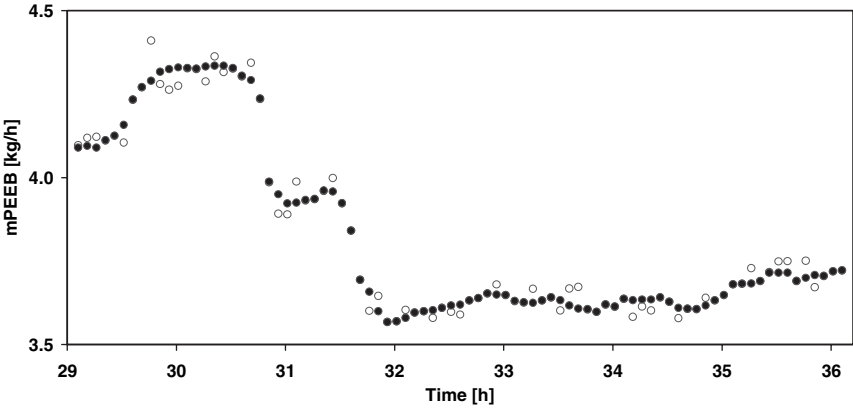


Figure 7.  
 $m_{PEEB}$ : Measured (○), reconciled (●).

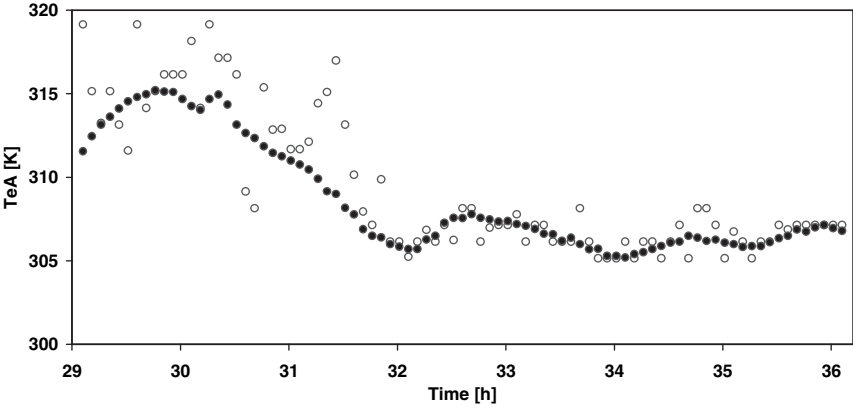
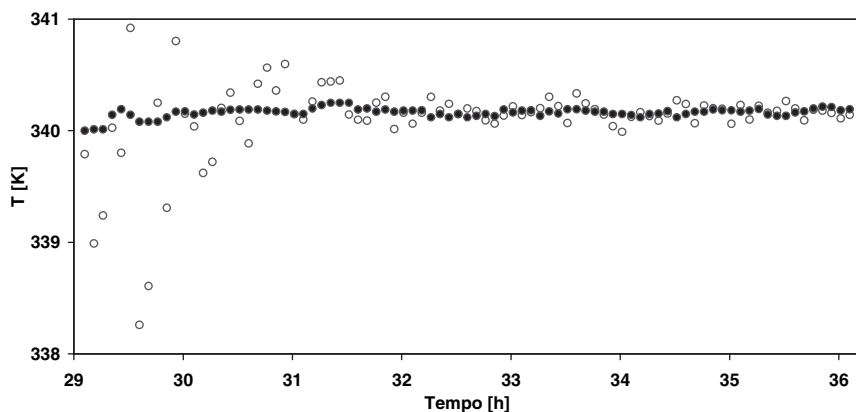


Figure 8.  
 $T_{eA}$ : Measured (○), reconciled (●).



**Figure 9.**

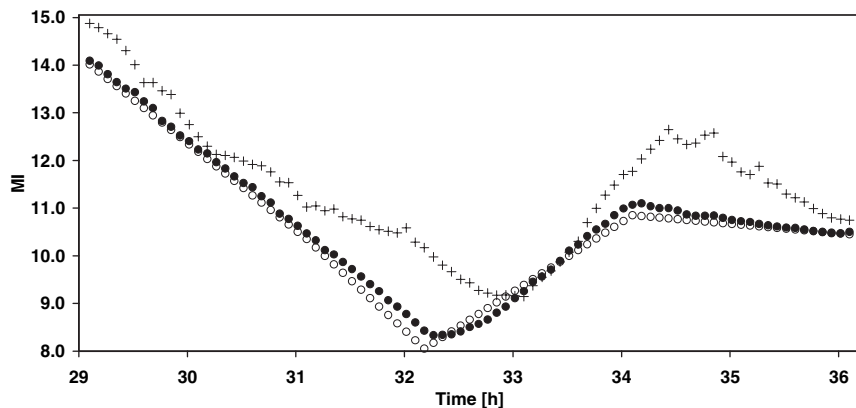
T: Measured (○), reconciled (●).

reflux propylene stream from the top condenser (A) and for the reactor temperature. In both cases very good filtering of measured data can be observed. The reconciled values seem to represent the actual process operation conditions much more accurately than the available measured data, given the much lower noise levels.

Finally, Figures 10 and 11 show the reconciled values of two important measured properties of the final product, *MI* and *XS*. Availability of reliable measurements of such properties in real time may be very important for the process operation and for

the process economics, as monitoring and control of polymer quality becomes possible for variables that are usually measured infrequently in the lab and only after product sampling. In both cases these values are compared with the ones obtained when no energy balance is considered. Again, inclusion of the energy balance leads to better results.

It is very important to note that the computational time required for the calculations of each window is about 40 s, a quite small value, if compared to the sampling time of 5 min. This clearly indicates that a further increase on the number of esti-



**Figure 10.**

MI: Measured (○), reconciled (●), reconciled without EB (+).

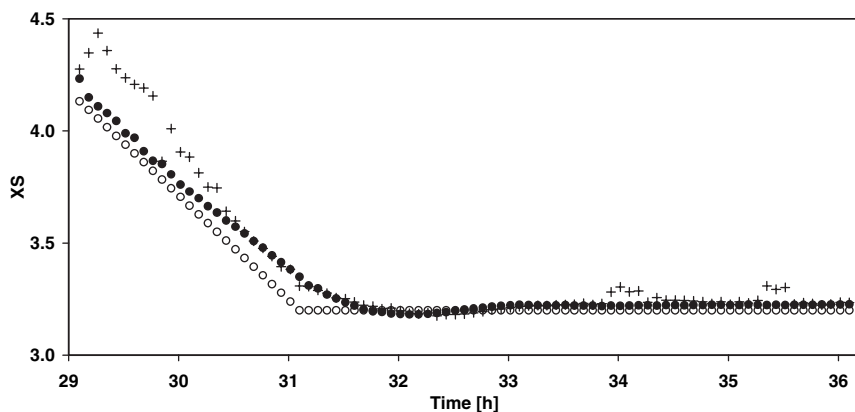


Figure 11.

XS: Measured ( $\circ$ ), reconciled ( $\bullet$ ), reconciled without EB (+).

mated parameters, non-measured variables and routines to deal with gross error detection is undoubtedly possible in-line, as desired. The computer used to perform the computations presented here was a standard Pentium 4 (3.0 GHz) with 1024 MB memory, which means that simultaneous data reconciliation and parameter estimation in a real polypropylene polymerization possible is indeed possible in standard desktop computers.

## Conclusions

In this work, an estimation technique for simultaneous on-line data reconciliation and parameter estimation has been implemented. An approach based on moving time window was used, and the resulting non-linear dynamic optimization problem was solved by a sequential strategy. The methodology was successfully applied to reconcile several sets of industrial data as well as to estimate non-measured parameters, like the ones associated to reaction productivity. It should be noted that the computational time required for the calculations on each sample period was a small fraction of such period, allowing for the on-line implementation of the algorithm. Results indicated that an increase of redundancy, using the energy balance

information, results in better reconciled and estimated values.

## Nomenclature

$C$ :	kinetic constant for transfer to hydrogen
$C_a$ :	propane concentration in the feed and recycle streams
$Cat$ :	mass of catalyst in the reactor
$C_{pa}$ , $C_{pe}$ , $C_{ppol}$ , $C_{pw}$ :	heat capacities of propane, propylene, polymer and water
$K_p$ :	kinetic constant for homo-propagation
$K_d$ :	catalyst deactivation constant
$K_0$ , $K_{xs}$ :	parameter
$L$ :	reactor volume
$M$ :	total mass in the reactor
$m_{bleed}$ , $m_{rec}$ :	liquid bleed and recycle flowrates
$m_{cat}$ , $m_e$ , $m_{PEEB}$ , $m_{TEA}$ :	input flowrates of catalyst, propylene, TEA and PEEB

$m_{eA}, m_{eB}$ :	reflux flowrates of propylene from top condensers	$w_{pol}$ :	polymer concentration in the slurry stream
$m_{pol}, m_{slurry}$ :	output polymer and slurry flowrates	XS:	xylene extractable material of the final resin
$m_w$ :	water flowrate of top heat exchanger	XS <sup>R</sup> :	xylene extractable material reference value
$M_n^I, M_n^{ac}$ :	instantaneous and cumulative number average molecular weights	$\alpha$ :	TEA recycle factor
$M_w^a$ :	cumulative mass average molecular weight	$\Delta H$ :	heat of reaction
MI:	melt index of the final resin	$\gamma$ :	parameter
N:	number of polymer mols	$\lambda$ :	parameter
Pa, Pe, PEEB, Pol:	masses of propane, propylene, PEEB and polymer in the reactor	$\lambda_e$ :	latent heat of vaporization of propylene
PD:	polydispersity	$\rho_a, \rho_e, \rho_{pol}$ :	densities of propane, propylene and polymer
PH <sub>2</sub> :	hydrogen pressure in the reactor	<p><b>Acknowledgements:</b> The authors thank CNPQ and CAPES for financial support. The authors also thank Suzano Petroquímica. S.A. for providing technical information and support.</p> <p>[1] D.R. Kuehen, H. Davidson, <i>Chem. Eng. Prog.</i> <b>1961</b>, 57, 44.</p> <p>[2] C.M. Crowe, <i>J. Proc. Cont.</i> <b>1996a</b>, 6, 89.</p> <p>[3] R.S.H. Mah, "Chemical Process Structures and Information Flows", Butterworth Publishers, Stoneham, MA, <b>1990</b>.</p> <p>[4] S. Narashimhan, C. Jordache, "Data Reconciliation and Gross Error Detection: An Intelligent Use of Process Data", Gulf Professional Publishing, Houston, TX, <b>2000</b>.</p> <p>[5] J.A. Romagnoli, M. C. Sanchez, "Data Processing and Reconciliation for Chemical Process", Volume 2 of Process System Engineering, Academic Press, 2002.</p> <p>[6] D.K. Rollins, S. Devanathan, M.V.B. Bascuñana, <i>Comput. Chem. Eng.</i> <b>2002</b>, 26, 1201.</p> <p>[7] C.M. Crowe, <i>Chem. Eng. Sci.</i> <b>1996b</b>, 51, 3359.</p> <p>[8] H. Tong, C.M. Crowe, <i>AIChE J.</i> <b>1995</b>, 41, 1712.</p> <p>[9] J. Chen, J.A. Romagnoli, <i>Comput. Chem. Eng.</i> <b>1998</b>, 22, 559.</p> <p>[10] P. Vachhani, R. Rengaswamy, V. Venkatasubramanian, <i>Chem. Eng. Sci.</i> <b>2001</b>, 56, 2133.</p> <p>[11] D.B. Öziurt, R.W. Pike, <i>Comput. Chem. Eng.</i> <b>2004</b>, 28, 381.</p> <p>[12] S. Cao, R.R. Rhinehart, <i>J. Proc. Cont.</i> <b>1995</b>, 5, 363.</p> <p>[13] I.W. Kim, M.S. Kang, S. Park, et al., <i>Comput. Chem. Eng.</i> <b>1997</b>, 21, 775.</p> <p>[14] M.J. Bagajewicz, Q. Jiang, <i>AIChE J.</i> <b>1997</b>, 43, 2546.</p>	
$R_{pol}$ :	rate of polymerization		
T:	reactor temperature		
TEA:	mass of TEA in the reactor		
$T_{eA}, T_{eB}$ :	temperatures in reflux flowrates of propylene from top condensers		
$T_{eis}, T_{erec}$ :	temperatures in input and recycle streams of propylene		
$T_{wis}, T_{wo}$ :	temperatures of input and output water streams from top heat exchanger		
V:	reactor volume		
$w_a$ :	propane concentration in the recycle stream		

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