Simultaneous Validation of Online Analyzers and Process Simulators by Process Data Reconciliation

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We present a model based algorithm for simultaneous validation of online analysers and process simulators. Reconciled on-line and historical process data satisfying balance and model equations provides the opportunity to validate and improve process models and soft sensors. Accurate simulation results and laboratory measurements can be used for the validation of online analysers. Validated and reconciled data can be used to the iterative and interactive identification of the unknown parameters of the simulator, e.g. for the determination of kinetic parameters. This method can also be used for monitoring and diagnostics of complex processes because situations when the operating conditions have been significantly changed can be discovered. The approach is illustrated by the analysis of an industrial hydrogenation system. We present the proposed iterative and interactive procedure of model development and analyser validation, the applied data reconciliation method, and the details of the case study. The results show the applicability of the proposed scheme in industrial environment and the benefits of the extracted information in the maintenance and monitoring of advanced model based process engineering tools. The developed tool can increase operating efficiency that is the key of reducing energy consumption and environmental impact. This is especially true in hydrocarbon industry where the operation of the technology is supported by process simulator and on-line analyser based advanced process control systems.

1. Introduction

Thanks to the evolution of information technology on-line and historical process data provides the opportunity to better understand the operation and malfunctions of chemical processes. The extracted information can be used for process monitoring to ensure consistent product quality. Collected data can also be used for the development and validation of process simulators that are often applied to improve industrial processes

Usually process simulators are based on first-principles (also referred as mechanistic, a priori, and white-box) models. These models consist of balance equations (mass, component, energy) representing detailed physical-chemical information about the system. Unfortunately, in many practical applications processes are often too complex and the related mechanisms are not sufficiently well understood for the successful application of this approach. Furthermore, the development of first-principle models of complex industrial process is very difficult and time-consuming procedure. In particular, it is difficult to build precise first-principle models that can explain why defects appear in products. This is a critical issue since product life cycles are getting shorter and the time available for improving of product quality and yield requires fast and adaptive solutions.

Data driven (black-box or a posteriori) model are built when no detailed knowledge is available about the process. In this case historical process data is used to build statistical models to determine the relationship between inputs and outputs. In the last decade these data-based approaches have been widely accepted.

Many companies have built integrated databases to store historical process data from all plants, process units and product properties. Statistical regression methods have also become increasingly popular techniques for process modelling and they are used for fault detection and quality estimation. However, measurements are always affected by errors affecting the quality of these models. One type of models is data reconciliation which is a procedure to calculate a minimal correction to measured variables, to make them verify a set of model constraints, such as material and energy balances (Kadlec, 2009).

A new direction is the combination simulators and data based statistical models that can handle random and gross errors (Kanoa, 2008). Thereby if measured data is processed in statistical models and it will be input of physical model, the simulator will give more reliable result.

The key idea of this paper is that simulator development and data reconciliation should be performed simultaneously. Firstly, raw data is reconciled based on a priori information based model. This reconsolidated data is used as an input of the process simulator. The unknown parameters of the simulator are also identified based on this for reconciled data. This improved model can be used again for reconciliation of the raw data. This procedure could be repeated till there is a significant difference between reconciled and calculated process values.

The applicability of the proposed approach is confirmed through an industrial case study related to the model development of a C3-hydrogenation system. Results show that flow measurements do not require significant correction. Based on simple component balances the quality of measurements provided by online analyzers can be significantly improved. This validated data can be used to determine reaction kinetic parameters (e.g. pre-exponential factor).

The structure of the paper is the following. The proposed methodology is presented in Section 2. The application example is given in Section 3. In Section 3.1 the technology and the motivation of model development are introduced. Most important results are presented and discussed in Section 3.2. Finally, Section 4 draws some conclusions.

2. Simultaneous validation of process data and mechanistic models

Process variables characterizing and influencing product quality has significant role in process control and optimization. Sometimes important variables cannot be measured in real time, because maybe it is too expensive or it can be occur due to lack of appropriate on-line instrumentation. Off-line laboratory tests mostly take more than two hours which time delay can cause control problems resulting economic loss. In such situations an improved monitoring system is required to online determine product quality. Sensor development is important task in chemical engineering (Zaouak, 2012). On-line analyzers eliminate the dependence on laboratory data can to support timely information for real time control. Unfortunately online measurements are less accurate and less reliable than lab measurements. Therefore the validation and reconciliation of the measurements of online analysers is also needed (Gidwani, 1994).

In our methodology simulation results (which satisfy balance equations) are compared to measured outputs and reconciled outputs (see Fig 1.). When there is significant difference between reconciled and calculated outputs, the unknown parameters of the simulator are re-identified based on the reconciled input and outputs. Based on reconciled data and re-identified parameters new simulation is elaborated and the reconciled and calculated outputs are compared again. Reconciliation and parameter estimation procedure continues while the difference between reconciled and calculated outputs is insignificant i.e. the reconciled data satisfies balance equations.
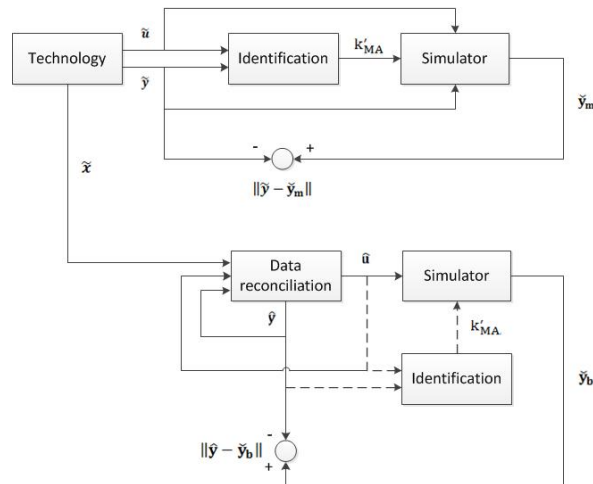
Figure 1: Iterative procedure for treating measurement error and developing simulator

Data reconciliation is a method to ensure that corrected data satisfy balance equations (Prata, 2009). Classical data reconciliation techniques are based on the projection of data into a linear hyperplane defined by the linear model of the system, $Ax = b$. The projection is optimal and applicable when the following assumptions are valid: (1) Measurement errors are independent from the balance variables. (2) Expected value of measurement errors is zero. (3) Measurement errors are in normal (Gaussian) distribution. (4) Errors of different measurement location are independent from each other (diagonal covariance matrix).

To formulate the problem let us consider an **x** vector containing the vector of inputs **u** and outputs **y**.

Reconciled values should satisfy balance equations and should be consistent with the values estimated by the process simulator. . Measured values are denoted by $\tilde{\ }$, reconciled variables by $\hat{\ }$; and results of simulator by $\breve{\ }$. The $\|\hat{y} - \breve{y}_b\|$ error indicates the success of the projection and consistency of the model used for prediction and the model used for process simulation. Both $\breve{y}_m$ and $\breve{y}_b$ depend on the parameters of the simulator. The aim is minimize initial this $\|\hat{y} - \breve{y}_b\|$ error and also the error between the measurement and the simulated values.

The classical data reconciliation is formulated by the following equation:

$$\hat{x} = \left(I - V_{\tilde{d}}A'\left(AV_{\tilde{d}}A'\right)^{-1}A\right)\tilde{x} + V_{\tilde{d}}A'\left(AV_{\tilde{d}}A'\right)^{-1}b \tag{1}$$
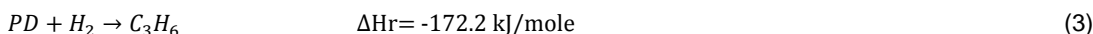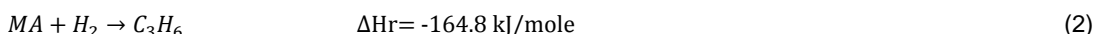
where $\tilde{x}$ contents the measured variables, **I** is an identity matrix, $V_{\tilde{d}}$ is the variance matrix of the error. The variances were determined by discrete Fourier transform. Fourier transform gives a graphical overview of the differences between basic process trends and noise in frequency domain. Based on the analysis of these spectra the parameter of a filter used to separate the noise from process trends can be determined. The whole procedure and the data reconciliation algorithm have been realized in MATLAB development environment.

3. Application to an industrial C3-hydrogenation system

Adequacy of proposed approach is applied in for model based development of a complex reaction system. In the first subsection technology is described then the results of reconciliation and simulation are introduced.

3.1 Description of technology

Tisza Chemical Group Plc. (TVK) is the largest petrochemical company of Hungary where polymer raw materials (ethylene, propylene, butylenes, etc.) are produced by steam cracking of naphtha or gasoline. At high temperature numerous free radical reactions occur. Some of them are undesirable due to poisoning catalysts of the following polymerization reactions (e.g. acetylene, methyl-acetylene, propadiene). Another problem is that these components are difficult to separate from the main products by distillation. Due to these problems these hydrocarbons are hydrogenised in a trickle-bed reactor used for the catalytic transformation of methyl-acetylene (MA) and propadiene (PD) to propylene.

$$MA + H_2 \rightarrow C_3H_6 \qquad\qquad \Delta Hr= \text{-164.8 kJ/mole} \qquad\qquad (2)$$

$$PD + H_2 \rightarrow C_3H_6 \qquad\qquad \Delta Hr= \text{-172.2 kJ/mole} \qquad\qquad (3)$$

The simplified flowsheet diagram of the process is depicted in Figure 2. The success of reactions is characterized by MAPD content measured by three online analyzers of raw C3 fraction (A1), inlet stream of reactor (A2) and diluting streams (A3).

The operation of the technology is supported by periodical laboratory measurements collected from two process streams (at Figure 2. these streams are denoted as L1 and L3. You can also see that there is no sampling before the reactor). Laboratory data is more accurate than online data so it has the potential for the validation of online analyzers and process models (identification of pre-exponential factor).
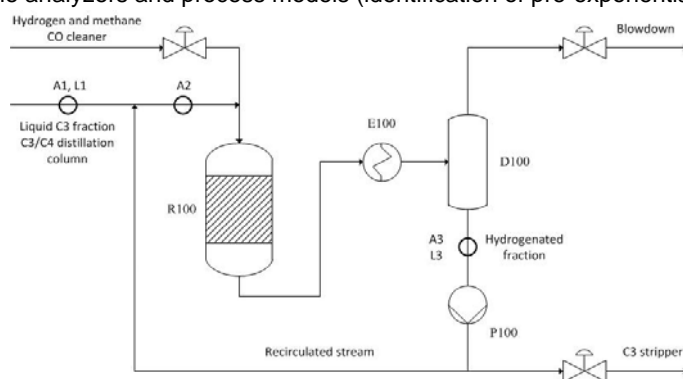

Figure 2: Process flowsheet diagram of C3-hydrogenation system

The key objective of this case study was to stabilize and improve the operation of this system. The analysis and optimization of the process requires not only accurate process simulator but accurate and valid measurements. The model used by the simulator can also be used to build a soft sensor and operator training system (OTS). Therefore, the main tasks of the project were the development of this simulator and validation of the online analyzers.

3.2 Results and discussion

Firstly we developed the process simulator in Aspen One software. For this purpose we analyzed all the characteristics of inlet streams, operating conditions and equipment of technology. Exception one parameter, all necessary data were collected from Olefin-2 plant of TVK Plc and from the scientific literature. The simulator of C3 hydrogenation system has been developed in Aspen Plus software. The developed Aspen Simulation Workbook framework allows the comparison of measured, reconciled data and calculated results.

Since hydrogen is dosed in excess, concentration of hydrogen is assumed to be constant. Thus, pre-exponential factor includes the dependence of hydrogen:

$$r_{MA} = k'_{MA} \cdot exp\left(\frac{-E_{a,MA}}{RT}\right) \cdot c_{MA} \qquad\qquad (4)$$

$$r_{PD} = k'_{PD} \cdot exp\left(\frac{-E_{a,PD}}{RT}\right) \cdot c_{PD} \qquad\qquad (5)$$

Concentration is in mole fraction unit, pre-exponential is in 1/s. In the literature (Gobbo, 2004) the activation energy is known for all reactions (Propadiene: 4,400 kJ/kmole, methyl-acetylene: 8960 kJ/kmole, propylene: 18,170 kJ/kmole), but pre-exponential factor is identified based on measured and reconciled data. The results are shown in Table 1.

Table 1: Estimated pre-exponential factor in case of different iterative steps

Basis of calculation	k'_{MA} (1/s)	Relative error
measured data	1.903	1.000
after first data reconciliation	3.445	0.1884
after second data reconciliation	3.812	0.0577

Figure 3 shows both measurements and simulation results. "First time" simulation is based on measured input data where the pre-exponential factor is identified based on the raw measured input-output data pairs. It is visible that the difference between measured and calculated output is significant. Following the proposed approach measured data is then reconciled based on the resulted model and new pre-exponential factor is estimated based on these reconciled data pairs. The difference between the simulation results and processed data is reduced (see second row of Table 1). After the second iteration the result is considered to be adequate because difference between the reconciled and calculated output is negligible and one more cycle does not resulted better solution.
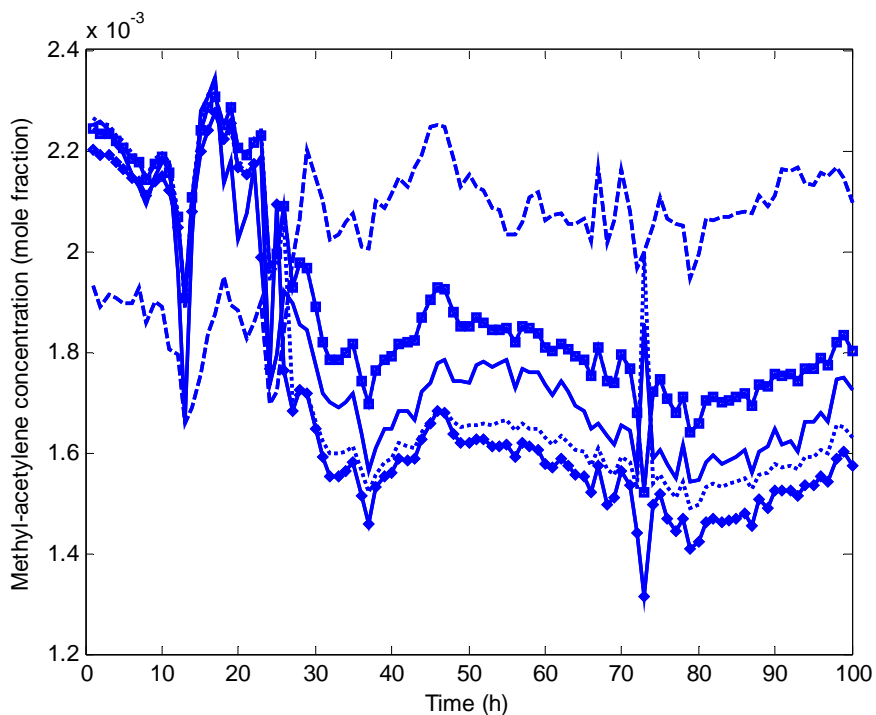

Figure 3: Comparison of measured, reconciled and calculated outputs. ——— measured output, ⋯⋯ after reconciliation, — — — simulated based on measured input data, —■— simulated based on reconciled input data (after first identification), —◆— simulated based on reconciled input data (after second identification)

4. Conclusion

Flowsheeting simulators are useful to support process operation and development. The success of these applications depends on the quality of the utilized model. Measurements used for the identification of unknown parameters of these models are always affected by errors. When model based data reconciliation techniques are applied more reliable data can be obtained. Hence, by using data reconciliation much more accurate and consistent simulator can be obtained from measured data. By following the proposed iterative approach not only better model was developed but the resulted information also contributed to the validation of online analyzers. The applicability of the proposed scheme has been demonstrated in industrial environment. Where the operation of the technology is supported by process simulator and on-line analyser based advanced process control systems the developed tool can increase operating efficiency.

Acknowledgements

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