CHEMICAL ENGINEERING TRANSACTIONS

VOL. 35, 2013

A publication of AIDIC
The Italian Association of Chemical Engineering
www.aidic.it/cet

Guest Editors: Petar Varbanov, Jiří Klemeš, Panos Seferlis, Athanasios I. Papadopoulos, Spyros Voutetakis

ISBN 978-88-95608-26-6; ISSN 1974-9791

DOI: 10.3303/CET1335082

Dynamic Data Reconciliation in a Hot-oil Heat Exchanger for Validating Energy Consumption

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Measured data from instruments are usually composed of errors. Data reconciliation is applied to improve the accuracy of measured data to satisfy mass and energy balances of the process. This work is focused on dynamic data reconciliation of a utility heat exchanger using hot oil from a waste heat recovery unit as a hot stream to heat up ethane product as a cold process stream from a natural gas separation plant. The measured data include flow rates, supply and target temperatures of hot oil and cold process streams. The dynamic data reconciliation was done by a combined optimization and constraint model solution strategy by converting the differential equations of the unsteady state equations to the algebraic equations using Euler's approximation. Adjustment of the hot oil flow rate of the fixed-area utility exchanger leads to a change in the target temperatures of the hot oil and cold process streams, as well as energy consumption. Excel's solver and commercial optimization software, General Algebraic Modelling System (GAMS), with a weighted least-square objective function are used for performing data reconciliation to validate the measured data and energy consumption. After data reconciliation was completed, estimates of process variables are more accurate and satisfy the process constraints.

1. Introduction

A modern chemical plant consists of a large number of process units, which are interconnected together by a complicated network of streams. Measurements of flow rates, temperatures, pressures, levels, concentrations of components and automatically recorded are routinely made for the purpose of process control, online optimization, or process performance evaluation. Measured process data are certainly corrupted by errors during the measurement. The total error in a measurement, which is the difference between the measured value and the true value of a variable, is represented as the sum of the contributions from two types of errors––random errors and gross errors.

Data reconciliation (DR) is a technique that has been developed to improve the accuracy of measurements by reducing the effect of random errors in data. This technique uses process model constraints and obtains estimates of process variables by adjusting process measurements so that the estimates satisfy the constraints (Narasimhan and Jordache, 2000).

The DR problem was first introduced by Kuehn and Davidson (1961) for linear steady-state models. As industrial processes are subject to regular changes, it is essential to reconcile process measurements in a dynamic scenario (Kong et al., 2000).Dynamic processes are commonly described by sets of nonlinear ordinary differential equations, which may contain model parameters and initial conditions that should be estimated from available plant data.The necessity of developing nonlinear dynamic data reconciliation (NDDR) methods was proposed by Liebman and Edgar (1998), and the advantages of using nonlinear programming over traditional steady-state DR methods were demonstrated. Liebman et al. (1992) developed their main NDDR algorithm. Their approach was based on simultaneous optimization and solution techniques where efficient state estimation was performed. In general, three classes of algorithms have been used to solve these NDDR problems (Kong et al., 2000; Dovi and Del Borghi, 2001): the extended Kalman filter (see, for

Please cite this article as: Singhmaneeskulchai P., Angsutorn N., Siemanond K., 2013, Dynamic data reconciliation in a hot-oil heat exchanger for validating energy consumption, Chemical Engineering Transactions, 35, 493-498 DOI:10.3303/CET1335082

example, Sirohi and Choi, 1996); artificial neural networks (see, for example, Karjala and Himmelblau, 1994); and constrained nonlinear programming. Dynamic constrained nonlinear programming consists of the optimization of a linear or nonlinear objective function, subject to nonlinear dynamic and algebraic constraints. The goal of this research is to use DR technique to remove the random errors from dynamic data of a hot-oil heat exchanger. DR technique use a weighted least-square objective function, based on the assumption that random errors follow normal distribution with zero mean and known variance. After DR is done, the energy usages of this heat exchanger were corrected and compared to the true values.

2. Physical system

The application of NDDR technique on a simulated dynamic hot-oil heat exchanger was demonstrated. The dynamic model for energy balance can be written as:

$$\frac{dQ}{dt} = \rho_o\, C_{p,o}\left[\left(T_{o,in} - T_{o,out}\right)\frac{dF_o}{dt} - (F_o)\frac{dT_{o,out}}{dt}\right] \tag{1}$$

$$\frac{dQ}{dt} = \left(F_{et}\,\rho_{et}\,C_{p,et}\right)\frac{dT_{et,out}}{dt} \tag{2}$$

$$\frac{dQ}{dt} = \frac{1}{6}UA\left(T_{o,in} - T_{et,out}\right)$$
$$\left[\left(T_{o,in} - T_{et,out}\right)\left(T_{o,out} - T_{et,in}\right)\frac{\left(T_{o,in} - T_{et,out}\right) + \left(T_{o,out} - T_{et,in}\right)}{2}\right]^{-2/3} \tag{3}$$
$$\left[-2\left(T_{o,out} - T_{et,in}\right)\frac{dT_{et,out}}{dt} + \left(T_{o,in} - T_{et,out} + T_{o,out} - T_{et,in}\right)\frac{dT_{o,out}}{dt}\right]$$

The Proportional Integral and Derivative (PID) controller equation to increase the hot oil flowrate (F_o) by changing set point (sp) can be written as:

$$\frac{dF_o}{dt} = \frac{1}{0.1}\left[\,1 + 0.7(sp - F_o) + 0.5Y - F_o\right] \tag{4}$$

$$\frac{dY}{dt} = (sp - F_o) \tag{5}$$

where Q is heat duty (W), F_o is volumetric flow rate of hot oil(m^3/h), $F_{et}$is volumetric flow rate of ethane product(m^3/h), $T_{o,in}$ is inlet temperature of hot oil (°C), $T_{o,out}$ is outlet temperature of hot oil (°C), $T_{et,in}$ is inlet temperature of ethane product (°C), $T_{et,out}$ is outlet temperature of ethane product (°C),U is overall heat transfer coefficient (W/m^2 °C), A is heat transfer area (m^2), and sp is set point. The physical constants for the model, which are not dependent on the operating conditions, are shown in Table 1.

Table 1: Physical data for dynamic hot-oil heat exchanger simulation

Parameter	Value	Units
$C_{p,o}$	2.4245	kJ/kg °C
$C_{p,et}$	2.3420	kJ/kg °C
ρ_o	778.15	kg/m^3
ρ_{et}	37.73	kg/m^3
U	310.6	W/m^2°C
A	46.1	m^2

3. Simulation data

This task involves simulating true values and measured values. True value is the value which assumes that the variable is directly measured without errors. Measured value is true value with random errors, like actual process data. There are eight process variables of a hot-oil heat exchanger which are F_o, F_{et}, $T_{o,in}$, $T_{o,out}$, $T_{et,in}$, $T_{et,out}$, U, and Q. True values were simulated at time step of 0.1 second over time period of 60 seconds obtained through numerical integration of the dynamic ordinary differential equations. Euler's approximation is one of the numerical integration used in this work. And then, 300 data are sampled at sampling time of 0.2 second. Measured values were obtained by adding Gaussian noise to sampled true values using Gaussian Random Number Generator through http://www.random.org/ to generate random numbers from a Gaussian distribution (a normal distribution). All measured variables are shown in Figure 1. These process variables are divided into two groups, steady and dynamic ones. Steady variables are F_{et}, $T_{o,in}$, and$T_{et,in}$. Dynamic variables are F_o, $T_{o,out}$, and $T_{et,out}$.

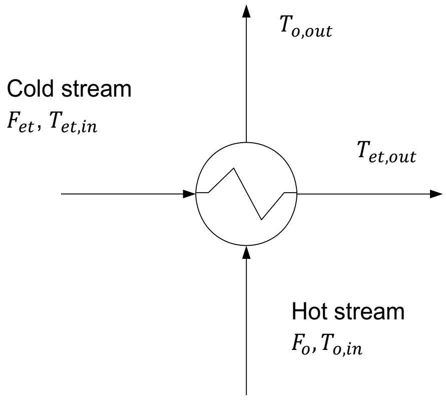

Figure 1: Variables in a hot-oil heat exchanger.

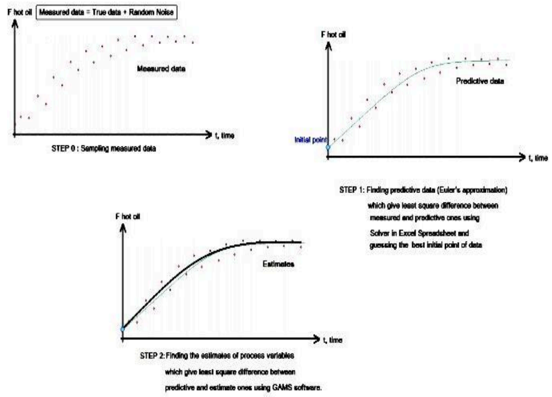

Figure 2: Dynamic data reconciliation steps.

4. Application of dynamic data reconciliation

First, measured process values were generated by adding random noise to the true values as shown step 0 in Figure 2. Next, Excel's solver was used to find initial and predictive values which minimize sum of the squared difference between measured value and predictive value; calculated from Euler's approximation as shown in step 1 in Figure 2.The reconciliation method used in this work is NDDR, originally developed by Liebman (1991). Gross errors are assumed as negligible (Yongkasemkul, 2012). This data reconciliation approach can be done on both steady and dynamic process as well as estimating parameters and unmeasured variables (McBrayer et al., 1998). The general NDDR problem can be written as:

$$Min\ \Phi\,(y(t), \hat{y}(t); \sigma) \tag{6}$$

subject to: $$f\left(\frac{d\hat{y}}{dt}, \hat{y}(t)\right) = 0 \tag{7}$$

$$h(\hat{y}(t)) = 0 \tag{8}$$

$$g(\hat{y}(t)) \geq 0 \tag{9}$$

where $\hat{y}(t)$ = estimates, y = discrete measurement, σ = measurement noise standard deviation, f = differential equation constraints, h = algebraic equality constraints, and g = inequality constraints

The measurement and estimate vectors include both measured states and inputs. The measurement noise standard deviations result from the reproducibility of each measurement device.
For most applications the objective function is weighted least-square:

$$\Phi(y(t), \hat{y}(t); \sigma) = \sum_{j=0}^{c} \frac{1}{2} (\hat{y}(t_j) - y_j)^T V^{-1} (\hat{y}(t_j) - y_j) \tag{10}$$

where $\hat{y}(t_j)$is the vector of values of the estimate functionsat discrete timet_j,$y_j$is the vector of measurementsat timet_j,$V$is the covariance matrix where each diagonal element, V_{ii}, and σ_i and $c$represents the current time. The off-diagonal terms can be assumed to be zero for most cases. Finally, weighted least-square objective function in GAMS model, as shown in step 2 in Figure 2, is used to minimize sum of the difference between mean of measured values and estimates for steady variable group, as shown in Eq(11). And the differences between predictive values (300 data) and estimates are minimized for dynamic variable group, as shown in Eq(11).

$$Min\left(\frac{F_{o,i}\,\rho_o\,C_{p,o}-\tilde{F}_{o,i}\,\rho_o\,C_{p,o}}{\sigma_{F_o}\,\rho_o\,C_{p,o}}\right)^2+\left(\frac{F_{et}\,\rho_{et}\,C_{p,et}-\tilde{F}_{et}\,\rho_{et}\,C_{p,et}}{\sigma_{F_{et}}\,\rho_{et}\,C_{p,et}}\right)^2+\left(\frac{T_{o,in}-\tilde{T}_{o,in}}{\sigma_{T_{o,in}}}\right)^2+$$
$$\left(\frac{T_{o,out,i}-\tilde{T}_{o,out,i}}{\sigma_{T_{o,out}}}\right)^2+\left(\frac{T_{et,in}-\tilde{T}_{et,in}}{\sigma_{T_{et,in}}}\right)^2+\left(\frac{T_{et,out,i}-\tilde{T}_{et,out,i}}{\sigma_{T_{et,out}}}\right)^2 \qquad (11)$$

The actual heat duty rate is calculated by energy balances; Eq(12), Eq(13) and Eq(14), for hot oil stream, ethane cold product stream, and heat exchanger, respectively. Eqs(15), Eq(16), Eq(17) and Eq(18) are inequality constraints for temperatures of hot oil and ethane product.

$$Q\;=F_{o,i}\,\rho_o C_{p,o}\,\Delta T_{o,i} \qquad (12)$$

$$Q\;=F_{et}\,\rho_{et} C_{p,et}\,\Delta T_{et,i} \qquad (13)$$

$$Q\;=UA(LMTD) \qquad (14)$$

$$T_{o,in}\;\geq\;T_{et,out,i} \qquad (15)$$

$$T_{o,out,i}\;\geq\;T_{et,in} \qquad (16)$$

$$T_{o,in}\;\geq\;T_{et,out,i} \qquad (17)$$

$$T_{et,out,i}\geq\;T_{o,in} \qquad (18)$$

Chen's approximation is used to calculate log-mean temperature difference as shown in Eq(19).

$$LMTD\;=\left[\left(T_{o,in}-T_{et,out}\right)\times\left(T_{o,out}-T_{et,in}\right)\times\frac{\left(T_{o,in}-T_{et,out}\right)+\left(T_{o,out}-T_{et,in}\right)}{2}\right]^{1/3} \qquad (19)$$

Degree of freedom (*dof*), the minimum number of pieces of information required in order to calculate all process variables is calculated from the difference between number of variables (including measured and unmeasured variables) and number of equations. Degree of redundancy (*dor*) is the difference between number of measured variables and degree of freedom. In the case of a hot-oil heat exchanger, degree of freedom is equal to 5 (*dof = 8 – 3 = 5*) and degree of redundancy is equal to 1 (*dor = 6 –5 = 1*). To perform data reconciliation, degree of redundancy must be greater than or equal to 1 (*dor* ≥ *1*). GAMS program is used to perform data reconciliation by minimizing the objective function (Eq(11))to estimate flow rates and inlet/outlet temperatures of hot oil and ethane product to satisfy process constraints (Eq(12) to Eq(18)).

5. Results and discussion

The dynamic hot-oil heat exchanger simulation was initialized at a steady operation of F_o = 39.38 m^3/h, F_{et} = 1,117.53 m^3/h, $T_{o,in}$ = 169.43 °C, $T_{o,out}$ = 103.21 °C, $T_{et,in}$ = 15.72 °C, and $T_{et,out}$ = 65.55 °C. The volumetric flow rate of hot oil was changed from 39.38 m^3/h to 100.0 m^3/h, resulting in a change in the outlet temperatures of hot oil and ethane product, as well as energy consumption. The estimates for the process variables, shown in Figure 3 to 9, show that estimates are closer to the true values than the measured values are, after performing data reconciliation.

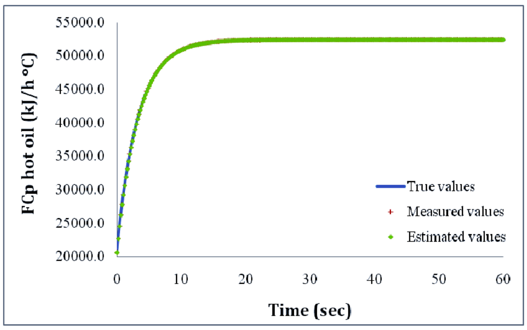

Figure 3: Set point change in volumetric flow rate of hot oil.

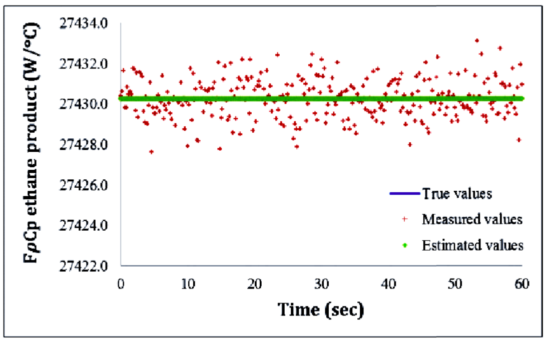

Figure 4: Ethane product volumetric flow rate estimate response to set point change in volumetric flow rate of hot oil.

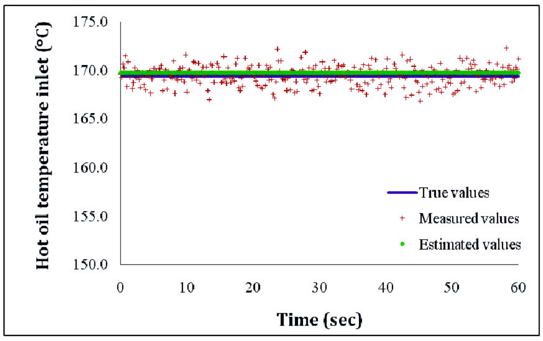

Figure 5: Hot oil inlet temperature estimate response to set point change in volumetric flow rate of hot oil.

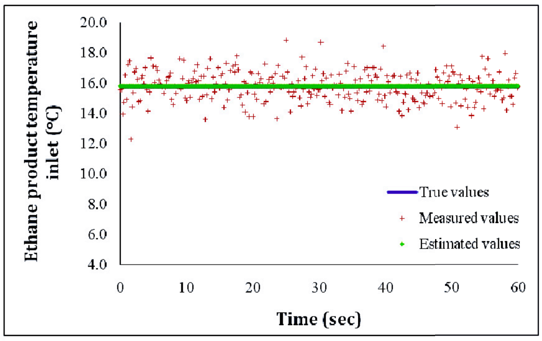

Figure 7: Ethane product inlet temperature estimate response to set point change in volumetric flow rate of hot oil.

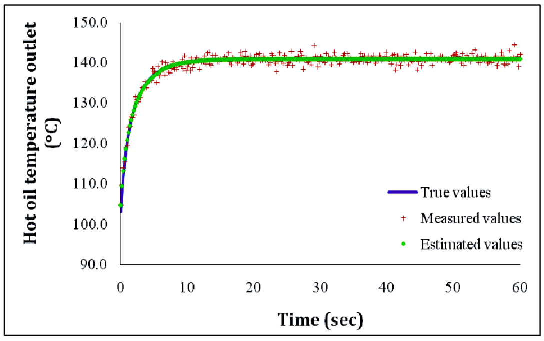

Figure 6: Hot oil outlet temperature estimate response to set point change in volumetric flow rate of hot oil.

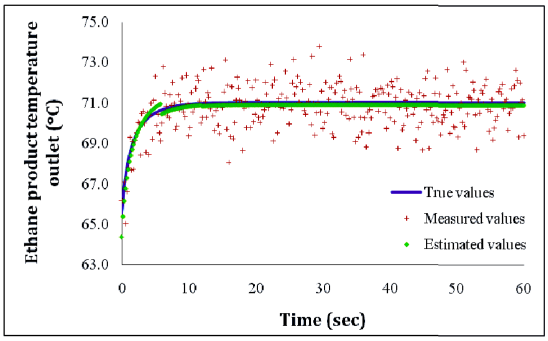

Figure 8: Ethane product outlet temperature estimate response to set point change in volumetric flow rate of hot oil.

A quantitative comparison between the estimates and the measured data confirming the qualitative results is presented in Table 2. After data reconciliation, standard deviations (SD) are decreased. These show the data had less variances meaning that most data are not deviated much from average ones. The smaller the standard deviations are, the more precise estimates are. The accurate estimates result in accurate heat duty and other process variables satisfying the constraint equations. Estimates of overall heat transfer coefficient (U) is 294.77 W/m^2 °C which is close to physical data of this heat exchanger.

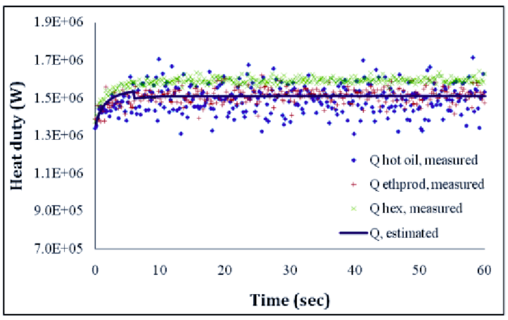

Figure 9: Heat duty estimate response.

Variable	Measurement Error Mean	Measurement Error SD	Estimate Error Mean	Estimate Error SD	%SD reduction
F_o	0.778	0.970	0.006	0.057	94.081
F_{et}	0.781	0.974	0.050	0.050	94.831
$T_{o,in}$	0.825	1.021	0.330	0.330	67.670
$T_{o,out}$	0.806	1.026	0.098	0.150	85.366
$T_{et,in}$	0.763	0.968	0.080	0.080	91.743
$T_{et,out}$	0.810	1.012	0.149	0.183	81.910

Table 2: Analysis of dynamic data reconciliation results

6. Conclusion

Dynamic data reconciliation of a hot-oil heat exchanger is presented in this work. The measured data including flow rates, inlet and outlet temperatures of hot oil and ethane product were simulated with random errors. The dynamic data reconciliation was done by a combined optimization and constraint model solution strategy with converting the unsteady differential equations to the algebraic equations using

Euler’s approximation. Increase in hot oil flow rate leads to increase in outlet temperatures of hot oil and ethane product, as well as energy consumption rate. Excel’s solver and commercial optimization software, General Algebraic Modeling System (GAMS), with a weighted least-square objective function are used for data reconciliation to validate the measured data and energy consumption. After data reconciliation was completed, estimates are more accurate satisfying the process constraints. The analysis of results shows that this approach provides accuracy from the reducing measurement mean, estimate mean, and error SD, in performing data reconciliation.

Acknowledgement

This work is funded by PTT Public Company Limited, The Petroleum and Petrochemical College, Chulalongkorn University, Thailand, Ratchadaphiseksomphot Endowment Fund and the National Centre of Excellence for Petroleum, Petrochemicals, and Advanced Materials, Thailand.

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