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Data Reconciliation for Total Site Integration

Jun Yow Yong*,[a], Andreja Nemet[b], Petar Sabev Varbanov[c], Zdravko Kravanja[b], Jiří Jaromír Klemeš[c]

[a]Faculty of Information Technology, University of Pannonia, Egyetem utca 10, 8200 Veszprém, Hungary
[b]Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ul. 17, SI-2000, Maribor, Slovenia
[c]Pázmány Péter Catholic University, Faculty of Information Technology and Bionics, Práter u. 50/A, 1083 Budapest, Hungary
junyow.yong@cpi.uni-pannon.hu

Data reconciliation is one of the important steps in Heat Exchanger Network (HEN) retrofit. Correctly performed data reconciliation can help in Heat Integration (HI) analysis. In this work, iterative method for reconciling heat exchanger network HI is explored. This work addresses the limitation encountered by the iterative method previously published. Several solution strategies have been evaluated. The work also proposes a procedure for data reconciliation at Total Site level. An illustrative case study shows the effectiveness of this iterative method. The iterative method provides a relatively good result, when compared with simultaneous method.

1. Introduction

It has been nearly 45 years since HI analysis has been introduced for energy recovery in chemical plants (Klemeš and Kravanja, 2013). The recent focus of HI has shifted on retrofitting existing chemical plant. The reason is that many existing HEN have become obsolete after years of service. With current fluctuating energy prices, increase production and change in process equipment, retrofitting can reduce operating cost with some investment. Various tools have been developed for this purpose. Yong et al. (2014) have developed a new tool to visually facilitate retrofit on single HEN, which is then extended by Yong et al. (2015a). Following up from the work, Yong et al (2015b) developed another HEN representation which uses matrix configuration. Nemet et al. (2015) proposed another representative diagram called Retrofit Tracing Grid Diagram, which clearly display the HEN into regions of heat exchangers, heaters and coolers according to the temperature scale.

Data Extraction (DE) is the very first and critical step performed before any HI study can commence (Klemeš, 2013). Particularly for existing plants, Data Reconciliation (DR) is a must in DE to obtain representative data (Klemeš and Varbanov, 2010). It is a procedure that extracts an accurate and reliable set of data from repeated raw measurements that satisfies the system constraints. Shenoy (1995) published a nonlinear programming model for HEN DR, based on average measurement values. Vocciante et al. (2014) developed a reconciliation strategy that assesses the convenience of using enthalpy balances in the reconciliation of flowrates. The resulting algorithm based in interval analysis provides a general framework on selection of equation to be used in reconciliation process. In the work of Kongchuay and Siemanond (2014), gross detection error technique is in DR to improve the data measurement of a simulated hot-oil heat exchanger using NLP.

The main HI analysis method – Pinch Analysis (PA), requires heat capacity flowrates (CP) and temperatures (T) of process streams. While there are already some publications on reconciliation of measured HEN data (Nemet et al., 2015), works presenting DE and DR for PA are scarce. The models proposed in the literature reconcile CP and T simultaneously. A non-simultaneous DR algorithm on HEN was introduced in the work of Ijaz et al. (2013). It involves using formulae to reconcile one parameter via QR factorisation. Although the algorithm is non-simultaneous, it is non-iterative as well. It reconciles one parameter at a time and stops after

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reconciling the last parameter. The algorithm first reconciles mass flowrates using only mass balance equations and then proceeds to reconciling measured temperatures using energy balance equations where the already calculated mass flowrate values are supplied as fixed parameters. As only mass balance equations are used in the first step of the algorithm, the mass flowrate values have influence on the result when temperatures are reconciled. However, the temperature values have no influence on the result when mass flowrates are reconciled.

To improve on this, the previous work by the current authors proposed an iterative method (Yong et al., 2016). Iterating between two sub-models, the method keeps one type of parameters constant (e.g. T) while reconciling the parameters of another type (e.g. CP), until satisfactory convergence is achieved. Two types of parameters are reconciled separately while still maintaining the importance of other parameters in the models. Although the iterative method features some inaccuracy, compared to the simultaneous method, it is can be significantly less computationally intensive and is simple to implement.

In this work, the iterative method for reconciling HENs is improved by addressing the limitation with over-specification encountered by the iterative method, as discussed in Yong et al. (2016). Several strategies are discussed to solve this limitation. The work also introduces an early attempt of DR at a Total Site level, without reconciling energy generated in any pressure changing equipment such as a steam turbine.

2. Iterative method and models

The HEN has non-linear system of constraints where temperature (T) and heat capacity (CP) are two parameters to be reconciled together. The complexity of the model increases with growing number of heat exchangers, causing more computational time needed. The first attempt to reduce the complexity is by assuming that mass flowrate is constant over time and specific heat capacity is independent on T. Consequently the value of CP is dependent on the mass flowrate. This reduces the system of constraints to bilinear in nature. In this work, the complexity is further reduced by using iterative method (Yong et al., 2016). The bilinear system of constraints is broken down in two sub-systems that use two linear models. These models are called T model and CP model. The T model assumes constant values for T in the constraints, and is solved to obtain values for CP. It is vice versa for CP model. The iterative method starts by using either model, as shown in step 3 in Figure 1. For example, if T model is chosen first, then mean T values are used in Eq(2) as shown in Figure 2. The obtained reconciled CP values are then used in the next step in CP model to obtain reconciled T values. This step is iterated until satisfactory results are obtained in these two parameters. The simultaneous is presented in detail in (Yong et al., 2016).

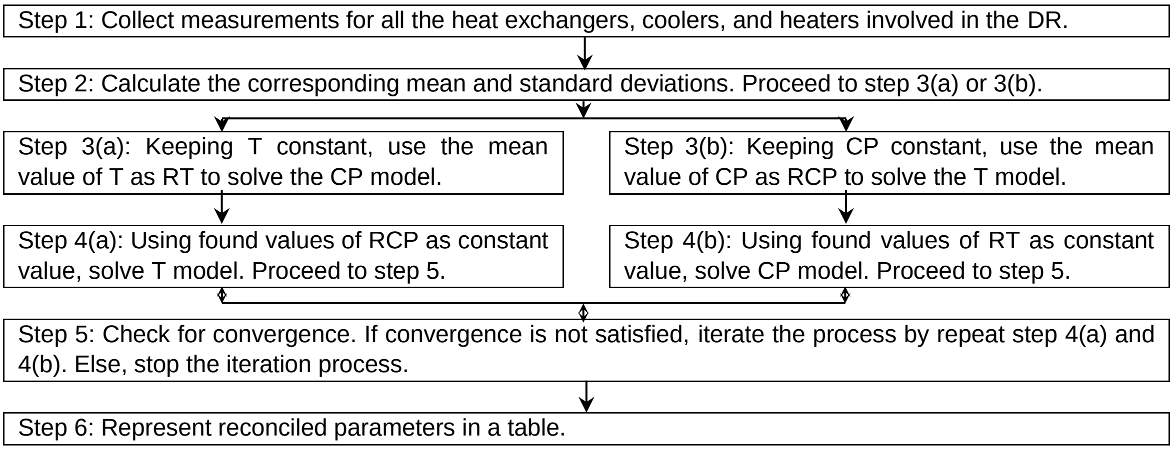
However, the iterative method has a limitation. Applied directly it is unable to reconcile HEN that has one or more heat loops. The simplest heat loop is two consecutive heat exchangers that are having same hot and cold streams. This is rather common in industries as heat load is too large to be performed by a single heat exchanger. It is usually designed to have two or more smaller heat exchanger. As the iterative method operates by assuming either one of the parameters to be constant, the problem becomes too constrained and infeasible. A few strategies are attempted to solve this limitation. Strategy 1 and 3 are used in this work. The results obtained from both strategies are compared:

1. Merging consecutive heat exchangers: The heat loads of such heat exchangers are combined in the model. The intermediate temperatures are calculated after the reconciliation. This is the simplest strategy but only applicable to consecutive heat exchangers and not to heat loops with multiple heat exchangers involves other streams.
2. Assuming these heat exchangers in heat loop with different CPs: The models allow heat exchangers in the heat loop to have different CPs. This is the most direct strategy. However, it is noted that using this strategy would cause difficulties in HI analysis particularly in PA. The value of CP of the stream is given in discrete instead of continuous manner, i.e. the CP suddenly “jumps” or “drops” when a certain temperature is reached. This forces the analysis to have the stream represented in two segments and hinders better HI.
3. Introducing a relaxation constant in every heat exchangers: Heat exchangers are relaxed to have difference in heat load instead. In the models Eq(5) is added with a relaxation constant - α as shown below. The relaxation constant, α has value between 0 and 1. The objective functions of both models also include α to be minimised. This strategy increases the computational load but it is still less than simultaneous method.

$$RCP_{s=HI,m}\left(RT_{s=HI,m} - RT_{s=HO,m}\right) = \alpha \times RCP_{s=CI,m}\left(RT_{s=CO,m} - RT_{s=CI,m}\right) \tag{6}$$

3. Illustrative Case Study

The case study is derived from Liew et al. (2012). In the case study, there are two chemical plants (A and B). PA shows that plant A requires minimum 2,250 kW and 400 kW of hot and cold utilities at 20 °C minimum temperature difference. While for plant B it requires minimum 100 kW and 1,543 kW of hot and cold utilities at 10 °C minimum temperature difference. The utilities available are cooling water (CW) from 15 °C to 20 °C, low pressure steam (LPS) at 133.6 °C, medium pressure steam (MPS) at 180 °C and high pressure steam (HPS) at 270 °C. Liew et al. (2012) performed Total Site HI analysis and found that available medium and LPS from plant B along with external 487.2 kW of LPS (EXLPS) can be supplied to plant A for heating. Figure 3 shows the HEN grid diagram with initial design values. Cooler A1, B1, B2 and B3 use CW. In Plant B, cooler B4, B7 and B10 generate LPS with hot streams from 190 °C to 143.6 °C. The coolers B5, B8 and B11 generate MPS with hot streams from 200 °C to 190 °C. As mentioned, the proposed model does not reconcile energy generated in steam turbine. Therefore MPS from plant B is assumed to be let down to LPS before sending to plant A. Measurements are taken over a period of time repeatedly 10 times for every heat exchanger in steady state. Six parameters are considered in every heat exchanger, namely inlet and outlet T for hot and cold streams (THI, THO, TCI and TCO) and CP for hot and cold streams (CPH and CPC). Table 1 shows an example of measurements taken for heat exchanger B9. With 21 heat exchangers with each 6 parameters to be measured, there are total of 126 parameters. The measurements for all other heat exchangers can be downloaded online (e.g. Google Drive). Table 2 shows the mean values of T and CP for all heat exchangers.



Step 1: Collect measurements for all the heat exchangers, coolers, and heaters involved in the DR.

Step 2: Calculate the corresponding mean and standard deviations. Proceed to step 3(a) or 3(b).

Step 3(a): Keeping T constant, use the mean value of T as RT to solve the CP model.

Step 4(a): Using found values of RCP as constant value, solve T model. Proceed to step 5.

Step 3(b): Keeping CP constant, use the mean value of CP as RCP to solve the T model.

Step 4(b): Using found values of RT as constant value, solve CP model. Proceed to step 5.

Step 5: Check for convergence. If convergence is not satisfied, iterate the process by repeat step 4(a) and 4(b). Else, stop the iteration process.

Step 6: Represent reconciled parameters in a table.

Figure 1: Algorithm of proposed iterative method

CP Model

$$Min \sum_{m}^{M}\sum_{s}^{S}\sum_{n}^{N} w_{s,m}\left(RCP_{s,m} - CP_{s,n,m}\right)^2 \quad (1)$$

where $W_{s,m}$ is the inverse of standard deviation of data measured. (Narasimhan and Jordache, 2000)
subject to:
Mass balance

$$RCP_{s=HI,m} = RCP_{s=HO,m} \quad (3)$$

$$RCP_{s=CI,m} = RCP_{s=CO,m} \quad (4)$$

Energy balance

$$RCP_{s=HI,m}\left(RT_{s=HI,m} - RT_{s=HO,m}\right) = RCP_{s=CI,m}\left(RT_{s=CO,m} - RT_{s=CI,m}\right) \quad (5)$$

where RT is assumed to be constant and constraints from the network

T Model

$$Min \sum_{m}^{M}\sum_{s}^{S}\sum_{n}^{N} w_{s,m}\left(RT_{s,m} - T_{s,n,m}\right)^2 \quad (2)$$

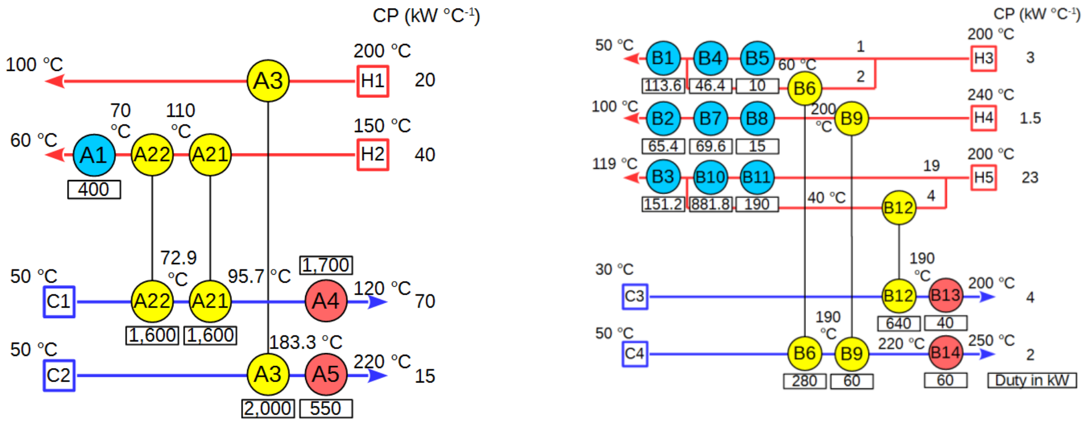
where $W_{s,m}$ is the inverse of standard deviation of data measured. (Narasimhan and Jordache, 2000)
subject to:

Energy balance

$$RCP_{s=HI,m}\left(RT_{s=HI,m} - RT_{s=HO,m}\right) = RCP_{s=CI,m}\left(RT_{s=CO,m} - RT_{s=CI,m}\right) \quad (5)$$

where RCP is assumed to be constant and constraints from the network

Figure 2: Models used in the algorithm



(a) (b)

Figure 3: Heat exchanger network Grid Diagram showing (a) Plant A and (b) Plant B used as DR case study at Total Site level. Note that values shown are initial design values

Table 1: Repeated measurement for heat exchanger B9

B9	THI	THO	CPH	TCI	TCO	CPC
1	240.1	199.5	1.48	189.5	220.3	2.03
2	239.8	200.4	1.49	189.7	219.9	1.95
3	239.8	199.7	1.53	189.6	220.3	1.98
4	239.8	200.4	1.46	190.1	220.1	1.95
5	240.5	200.0	1.50	190.5	220.1	1.98
6	239.6	200.1	1.54	189.5	220.5	2.03
7	240.3	200.2	1.46	190.4	219.7	2.04
8	239.8	200.0	1.51	189.9	220.4	2.02
9	239.7	200.4	1.54	189.6	220.4	2.01
10	239.5	199.9	1.48	190.4	219.7	1.96

Table 2: Mean values of T and CP for all heat exchangers

HEX	THI	THO	CPH	TCI	TCO	CPC
A1	70.05	60.06	40.07	14.92	19.87	79.93
A21	150.21	110.02	39.89	72.87	95.60	70.05
A22	110.16	70.03	40.01	50.10	72.90	70.01
A3	199.79	99.99	19.98	49.96	183.60	14.85
A4	133.60	132.60	1,702.30	95.76	120.19	70.03
A5	270.00	269.00	549.80	183.30	219.96	15.24
B1	87.79	49.94	2.98	15.04	20.04	22.68
B2	143.54	100.01	1.50	14.87	19.92	13.06
B3	125.60	118.85	22.90	14.91	19.94	30.34
B4	190.01	143.46	0.98	132.59	133.59	46.45
B5	200.01	189.88	1.00	179.00	180.00	9.97
B6	199.81	60.03	1.91	49.87	190.08	2.01
B7	189.99	143.40	1.50	132.59	133.59	69.79
B8	199.69	190.02	1.49	179.00	180.00	14.96
B9	239.89	200.06	1.50	189.92	220.14	2.00
B10	189.92	143.48	19.12	132.59	133.59	881.80
B11	199.98	190.16	19.10	179.00	180.00	189.60
B12	199.97	39.93	4.02	30.00	189.99	4.01
B13	270.00	269.00	39.98	190.08	199.96	4.02
B14	270.00	269.00	59.92	219.92	250.12	2.01
EXLPS	133.60	132.60	487.10	100.00	101.00	487.10

4. Results and Discussion

DR has been performed on the case study using three different methods; simultaneous method, iterative method employing strategy 1 and iterative method employing strategy 3.

Table 3: Number of parameters to be reconciled for each model

Methods	Simultaneous	Iterative Method (Strategy 1)		Iterative Method (Strategy 3)	
		CP Model	T Model	CP Model	T Model
No. of parameters	126	42	84	63	105
Sum of square error	580.74	961.9 (2nd iteration)		597.6 (2nd iteration)	
Simulation time (s)	3	1		1	

As shown in Table 3, the simultaneous method has more complex model and requires more computational effort as it has to reconcile 126 parameters simultaneously, while it is less for iterative method. The percentage difference for 126 reconciled parameters for each method is calculated by comparing with respective mean values. Figure 4 shows only parameters with significant percentage difference when compared among these three methods. That is all three methods have 84 parameters reconciled having percentage difference less than 0.10 %. Overall from Figure 4 it can be observed that simultaneous method has the best reconciled data followed by iterative method employing strategy 3 and then strategy 1. Reconciling data using simultaneous method on the case study has 123 parameters less than 1 % difference, whereas for strategy 3 and strategy 1 are 115 and 100 parameters. It should be noted that the simulation time presented is a rough estimation, it depends on the specification of the computer and solver used and size of the problem.

Although both are iterative method, employing strategy 3 is having better result than strategy 1. This is due to the introduction of relaxation constant, α in strategy 3. In the case study, 20 heat exchangers have relaxation constants close to 1. As expected, heat exchanger A21 has the largest relaxation constant at 0.983. This means that heat load of heat exchanger A21 at hot side is 1,566.3 kW while at cold side is 1,593.0 kW. The difference is 26.7 kW, or 1.675 % difference. This value is negligible when compared with total heat load. The introduction of relaxation constant in strategy 3 improves without heavy compromise on the result.

Overall, simultaneous method is still performing better than iterative method. However, considering the simplicity of the iterative methods models, iterative methods are preferred as they still provide feasible and relatively good results. As constrain equations used in iterative method is MILP, it can be run on free solvers such as Microsoft Excel as they are more robust. The results obtained from an iterative method can also be used as the starting point or initial guess for simultaneous method.

5. Conclusions

In this work, the limitation of iterative methods suitable for PA has overcame successfully with employing two strategies. Strategy 3 discussed in the work is able to overcome the limitation of any HEN having heat loop, which is discovered in previous work. Strategy 1 has simpler assumption but it is only usable on consecutive heat exchangers. Using iterative methods from reconciling illustrative case study in this work shows that it gives relative good result. The results also show that simultaneous method provides the best result, in expense of higher computational effort. The decision of using either simultaneous method or iterative method lies on the purpose of the DR. If the small errors are required and computational effort can be compromise, then simultaneous method is the choice. However, if the reconciled data is just for initial analysis where higher margin of error can be tolerated, then iterative methods can be used to obtain the result in much faster way. The results obtained from the iterative method can also be used as the initial input for simultaneous method, hence reduce the search time. This work also presents DR at Total Site level. Iterative methods show that it can be also reconcile steam flowrates. In future work, the complexity-precision trade-off for the two approaches should be quantified and hierarchical decomposition should be considered.

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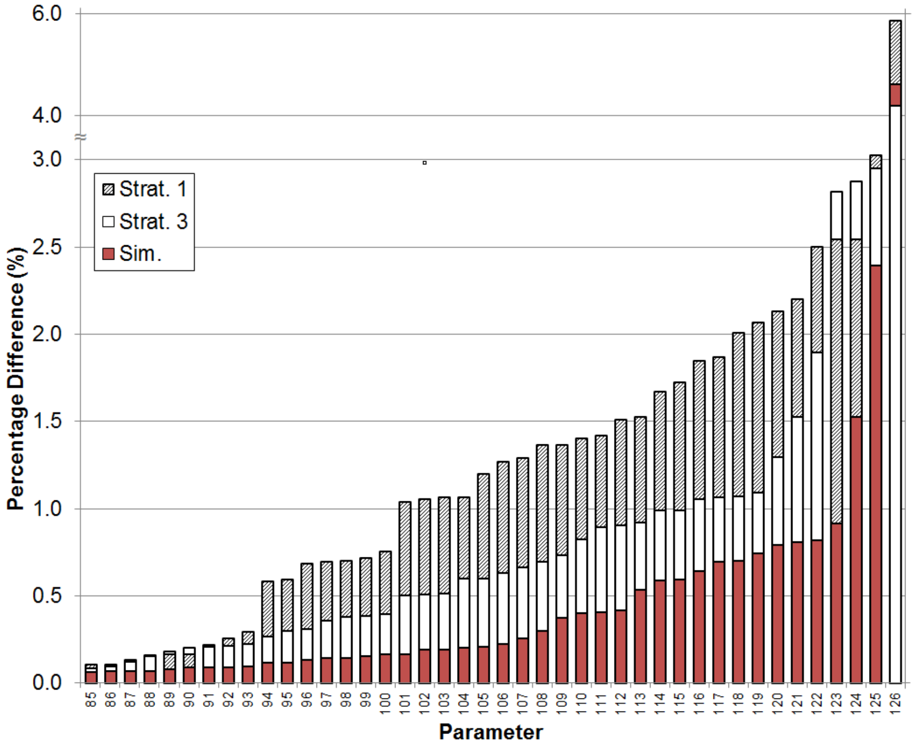

Figure 4: Percentage difference by comparing with respective mean values among various methods used. Please note that the 126th entry uses the right scale.

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