

Shortcut Data Reconciliation Technique: Development and Industrial Application

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Introduction

Software are being developed for industrial application to address the issue of data reconciliation either offline or online. These software are not commonly used by plant engineers because of either unavailability of the software, lack of time, or difficulties of configuring and maintaining the software. Nonetheless, plant engineers routinely require the use of consistent data sets to develop and validate process models for debottlenecking and improvement purposes. Even though many data reconciliation techniques are rigorously developed, a simple shortcut procedure to reconcile process data is lacking. The development of a simple yet systematic procedure for plant engineers to reconcile plant data is desirable.

The objective of this work is to develop a steady-state shortcut procedure to reconcile flow rate and concentration data. The procedure is easy to implement and the results are close to the optimum solution obtained by rigorous methods. Two cases drawn from industry are used to demonstrate the application of the procedure.

To verify the shortcut procedure reliability, the Q-R factorization approach¹ is used and the results of both approaches are compared. At this stage, the procedure assumes that the data do not contain gross errors. This assumption is made to keep the procedure simple without severely affecting the accuracy of the method. The Q-R approach is used to factor the unmeasured constraint matrix. The factorization decouples the unmeasured variables from measured ones. In general, the plant mass balance based on component flow rate may be written as

$$\mathbf{A}_1\mathbf{x} + \mathbf{A}_2\mathbf{u} = \mathbf{C} \quad (1)$$

where \mathbf{x} is a vector of the measured variables, \mathbf{u} is a vector of the unmeasured variables, \mathbf{C} is a vector of constants required in

the mass balance and/or just determined variables, \mathbf{A}_1 is the constraint matrix of the measured variables, and \mathbf{A}_2 is the constraint matrix for the unmeasured variables. The procedure to apply the Q-R approach to obtain the reconciled values is discussed in detail in Romagnoli and Sanchez¹ and Narasimhan and Jordache.² Some industrial applications are discussed in the literature.^{4,5}

Shortcut Data Reconciliation Technique

Typically, data are collected periodically, depending on the sampling time, and subsequently stored for retrieval. The data are usually averaged on a daily basis. The process is assumed to be in steady state and a minimum of 15 measurements for each variable should be available to provide reliable estimates of the variable statistical information.³ The shortcut procedure is the following:

(1) Identify key units and streams that are essential for development of the model.

(2) Reduce the process flow sheet complexity by combining streams, units, or components.

(3) Identify:

(a) All measured and unmeasured variables. Unmeasured variables could be process variables or quantities that need to be estimated.

(b) The major reactions and the components involved in these reactions. The involved components will be referred to as "active" reactive components.

(c) Other minor reactions and the components involved in these reactions. The involved components will be referred to as "pseudo" reactive components.

(4) Calculate the component flow rate from the total flow rate and composition measurements. Either mass or mole flow rates may be used with preference given to mole flow rate in systems with reactions.

(5) Estimate the average of each component flow rate (\bar{n}) and the standard deviation (σ) of the component flow rate calculated in step (4). Reject data that are greater than $\bar{n} + \sigma$

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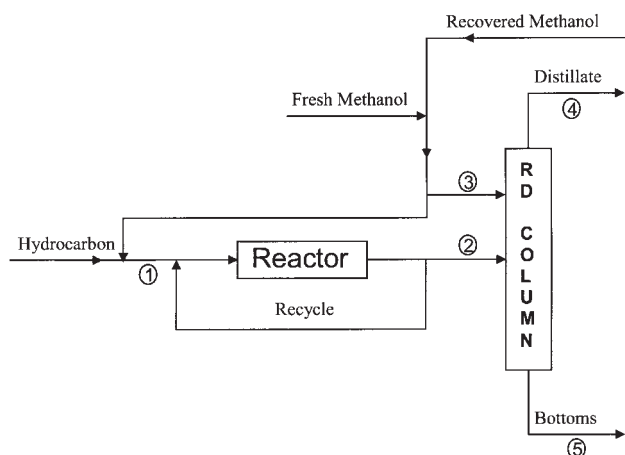


Figure 1. Process block diagram.

and less than $\bar{n} - \sigma$. Estimate the variance for each of the reduced data sets. This will be the diagonal element of the variance-covariance matrix. The off-diagonal elements are zeros.

(6) For nonreactive components:

(a) Component flow rate must be conserved and thus the reconciled component flow rate is the average of all the component's flow rates in the entire flow sheet.

(b) If the component is going through a mixer or a splitter (separator), the total flow rate is determined as discussed in step (6a), whereas the ratio of the component flow rates (the feed streams in mixers or the product streams in splitters) is the same as that obtained from the average of the reduced data in step (5).

(7) For reactive components:

(a) Pseudo reactive: treat these components as nonreactive before and after the reactive unit similar to step (6). The reconciled values for the input or output component flow rates are the average of all the component flow rates before or after the reactive unit unless another reactive unit is faced; then only the segment between the two reactive units is considered. The extent of minor reactions where these components are involved is computed from the reconciled input and output component flow rates. The computed extents of minor reactions are used in the minimization problem as just determined variables, that is, vector \mathbf{C} in Eq. 1. Mass balance as well as the computed extents of reactions are used to calculate other pseudoreactive components.

(b) Active reactive: use the Q-R approach for linear systems to find the reconciled component flow rates and to estimate the extents of the main reactions. This is done for the main reactions and the components involved in them.

(8) Determinable unmeasured nonreactive or reactive component flow rates as well as other unmeasured quantities are estimated as a by-product of steps (6) and (7) together with the mass balance equations. If desired, calculate the total flow rate and the composition of each stream from the reconciled component flow rates.

This procedure does not require developing special software. To apply this technique, one would need a spreadsheet program (such as Microsoft Excel) and mathematical program (such as Matlab). Both of these programs are readily available.

Although flow sheet reduction and variables classification might appear to be time consuming, plant engineers would find this easy to implement because of their field experience.

Description of the Industrial Process

Methyl-*tert*-butyl-ether (MTBE) is produced in industry through various schemes, one of which is through the use of reactive distillation technology. The process consists of a reactor section followed by reactive distillation. The process block diagram is shown in Figure 1. The process has 17 components: methane (C_1), ethane (C_2), propene (C_3^-), propane (C_3), isobutane ($i-C_4$), *n*-butane ($n-C_4$), 1-butene (1B), isobutene (IB), 1,3-butadiene (1,3-BD), 1-pentene (C_5), *n*-hexane (C_6), water, methanol (MeOH), *tert*-butyl alcohol (TBA), MTBE, methyl secondary-butyl ether (MSBE), and di-isobutene (DIB). The complete set of reactions that take place in the process is therefore



The last reaction is instantaneous and, thus, whenever water is present it will be converted completely to TBA. Around 30 measurements were available for each measured variable over a period where the process is believed to be at steady state.

Results and Discussion

In the shortcut approach, the basis for calculation is component mass balance. These component flow rates are the variables to be reconciled. This will render the reconciliation problem linear and thus easier to solve; however, the resulting reconciled data will be suboptimum because some of the variability in measurements will be altered as a result of the multiplication of the two measurements, that is, total flow rate and composition. This is a trade-off between accuracy and ease of use, which is acceptable in shortcut methods. The shortcut approach is implemented in two cases as discussed below.

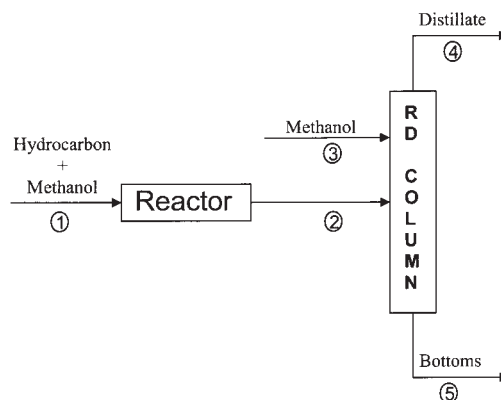


Figure 2. Reduced process block diagram.

Table 1. Results of Shortcut Approach vs. Q-R Approach for Cases 1 and 2*

Variable	Measurement (kmol/h)	Case 1			Case 2		
		Shortcut	Q-R	R.E.	Shortcut	Q-R	R.E.
Stream 1	Total	4236.90			4214.63	4244.77	0.71
	Methane				10.21	10.38	1.70
	Ethane				2.14	2.28	6.08
	Propene	9.08	9.10	9.53	4.57	9.07	9.53
	Propane	22.41	20.58	20.76	0.87	20.58	20.74
	Isobutane	1205.22	1170.50	1196.53	2.18	1170.50	1192.49
	<i>n</i> -Butane	30.07	29.11	29.22	0.38	29.06	29.19
	1-Butene	70.78	59.23	55.04	7.62	59.52	55.27
	Isobutene	1498.63	1479.81	1484.91	0.34	1477.75	1483.50
	1,3-Butadiene	9.21	8.31	8.00	3.77	8.31	8.00
	<i>i</i> -Pentene				0.71	0.60	18.48
	C6's+				8.78	9.33	5.91
	Water				1.59	1.77	10.04
	MeOH	1392.92	1419.52	1424.07	0.32	1416.42	1421.69
	MTBE						
	MSBE						
	TBA						
	DIB						
Stream 2	Total	2920.06			2900.07	2924.48	0.83
	Methane	9.66			10.21	10.38	1.70
	Ethane	2.22			2.14	2.28	6.08
	Propene	9.46	9.10	9.53	4.57	9.07	9.53
	Propane	20.36	20.58	20.76	0.87	20.58	20.74
	Isobutane	1156.82	1170.50	1196.53	2.18	1170.50	1192.49
	<i>n</i> -Butane	28.66	29.11	29.22	0.38	29.06	29.19
	1-Butene	49.90	59.23	55.04	7.62	59.09	54.90
	Isobutene	154.78	158.21	159.36	0.72	160.53	159.20
	1,3-Butadiene	8.72	8.31	8.00	3.77	8.31	8.00
	<i>i</i> -Pentene				0.71	0.60	18.48
	C6's+	8.59			8.78	9.33	5.91
	Water						
	MeOH	111.13	104.14	107.33	2.97	106.54	107.53
	MTBE	1354.05	1315.38	1316.74	0.10	1309.45	1313.79
	MSBE				0.43	0.37	16.53
	TBA	2.15			1.59	1.77	10.04
	DIB	3.73	3.11	4.41	29.55	3.09	4.37
Stream 3	Total	56.86			57.01	57.73	1.26
	MeOH	56.86	57.85	57.65	0.35	57.01	57.73
Stream 4	Total	1470.56			1440.69	1463.18	1.54
	Methane	10.66			10.21	10.38	1.70
	Ethane	2.30			2.14	2.28	6.08
	Propene	9.69	9.10	9.53	4.57	9.07	9.53
	Propane	21.07	20.58	20.76	0.87	20.58	20.74
	Isobutane	118.29	1170.50	1196.53	2.18	1170.50	1192.49
	<i>n</i> -Butane	28.80	28.15	28.20	0.18	28.10	28.17
	1-Butene	55.29	59.23	55.04	7.62	59.09	54.90
	Isobutene	74.72	72.60	72.38	0.31	70.15	71.98
	1,3-Butadiene	7.58	8.31	8.00	3.77	8.31	8.00
	<i>i</i> -Pentene						
	C6's+						
	Water						
	MeOH	74.16	65.72	64.58	1.76	62.54	64.70
	MTBE						
	MSBE						
	TBA						
	DIB						
Stream 5	Total	1444.83			1427.54	1432.12	0.32
	Methane						
	Ethane						
	Propene						
	Propane						
	Isobutane						
	<i>n</i> -Butane	1.02	0.96	1.02	5.83	0.96	1.02
	1-Butene						
	Isobutene						
	1,3-Butadiene						
	<i>i</i> -Pentene	0.59			0.71	0.60	18.48
	C6's+	9.43			8.78	9.33	5.91
	Water						
	MeOH	14.06	13.70	13.96	1.89	13.68	13.96
	MTBE	1413.05	1397.96	1403.17	0.37	1396.77	1400.40
	MSBE	0.37			0.43	0.37	16.53
	TBA	1.63			1.59	1.77	10.04
	DIB	4.69	4.62	4.68	1.26	4.62	4.67
Reaction extents in reactor	Rx 1		1315.38	1316.74	0.10	1309.45	1313.79
	Rx 2		3.11	4.41	29.55	3.09	4.37
	Rx 3				0.43	0.37	16.53
	Rx 4				1.59	1.77	10.04
Reaction extents in RD column	Rx 1		82.57	86.43	4.46	87.31	86.61
	Rx 2		1.52	0.27	453.60	1.54	0.30

*Key: Not considered in Case 1; not measured; not present in stream.

Case 1

To simplify the problem and examine the shortcut procedure in a smaller problem, the number of components is reduced by excluding the following components: C_1 , C_2 , C_5 , C_6 , water, MSBE, and TBA. In addition, only the main reaction and the DIB formation are considered. To apply the shortcut procedure, first we identify the key units as the reactor and the reactive distillation column. The key streams are numbered from 1 to 5 as shown in Figure 1. Based on this identification, the process flow sheet is reduced to reflect the key units and streams as shown in Figure 2. The reduced flow sheet is the “effective” process model whereby any improvement or debottlenecking to this reduced flow sheet will directly improve the overall process. All flow rates and compositions of concern in this model are measured. Table 1 identifies the measured and unmeasured variables. Based on the experience in this process and the data available, the major reactions are the MTBE and DIB formation reactions and, consequently, IB, MeOH, MTBE, and DIB are the “active” reactive components and thus no “pseudo” reactive components are considered in this case.

To verify the reliability of this procedure, its output is compared to that obtained from solving the complete problem using the Q-R approach. In the latter, the component flow rates were not filtered by omitting those data outside the range of $\bar{n} \pm \sigma$ and the Q-R minimization problem includes all components (reactive and nonreactive). In addition, the constraints include both the component balance and the total mass balance around each unit. In the shortcut approach the problem is to solve for 12 measured variables and four unmeasured variables subject to eight equations, whereas in the Q-R approach the problem has 36 measured variables and four unmeasured variables subject to 25 equations. One can immediately appreciate the reduction in the size of the problem when the shortcut approach is used. The relative error (R.E.) of shortcut method compared to the Q-R approach is shown in Table 1.

Case 2

In this case, all the components and reactions are considered. There are 46 measured variables and 13 unmeasured quantities, as shown in Table 1. The major reactions are the MTBE and DIB formation and IB, MeOH, MTBE, and DIB are the “active” reactive components. Formation of MSBE and TBA constitutes minor reactions and thus IB, TBA, MSBE, and water are “pseudo” reactive. The reconciled component flow rate of IB, for instance, before the reactor section is the average from the reduced set of the component flow rate before the reactor, whereas that after the reactor is the average of the reduced set of IB flow rate after the reactor and IB flow rate in the distillation column overhead. Because the TBA formation reaction is fast, the water in the feed is the same as the TBA in

the reactor product, and because MSBE is not measured after the reactor, its reconciled flow rate is the average of its distillation bottoms flow rate. The remaining variables are the “active” reactive components which are IB, MeOH, MTBE, and DIB. By using the Q-R approach, 12 measured variables, four unmeasured quantities, and two just determined quantities (extent of minor reactions) are subject to eight component mass balance equations. Similar to Case 1, the Q-R approach is applied to the full-scale problem where 46 measured variables and 13 unmeasured variables are subject to 38 constraint equations. The results of the shortcut and Q-R approaches are given in Table 1.

Conclusions

The performance of the shortcut approach compared to the rigorous Q-R approach is very good. In Case 1, <6% of the variables have a relative error >10%, whereas in Case 2 only 9% of the variables exceeded that level. For a shortcut approach we are not aiming for optimum solution but to get close enough to the optimum with a simple procedure. If we consider the Q-R approach to be an optimum solution then having >91% of the variables within a range of 10% from the optimum solution is considered very good from the perspective of a shortcut approach. Even though both approaches agree on the overall DIB formation, they differ in the formation ratio between the reactor section and the reactive distillation. The DIB measurement has substantial variability and, because the shortcut approach filters it out, the DIB value used in both approaches was different, which resulted in this difference in the formation ratio.

Acknowledgments

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