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Reconciliation of data with non random errors

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ABSTRACT

Errors in measured data could impact the offline optimizations or online control systems, leading to potentially uneconomical or unsafe process conditions. To address this issue, data reconciliation methods are introduced to enhance the data as much as possible. In this regard, the existence of non-random errors is challenging. This article debates the use of conventional sum of squares objective function in the case of presence of non-random errors. It shows how a robust estimator such as the maximum likelihood ameliorate the reconciliation. The robustness of the new objective function was assessed using simulated data. Results indicate that the sum of errors between real simulated data of flowrates and their estimation counterparts decreases from 124% to 27% in the case of a gross error in one stream, when robust objective function is manipulated. Even if no non-random error exists, it is shown that robust estimator could result in better data reconciliation, if optimum parameters are chosen for the robust objective function.

KEYWORDS

Data Reconciliation, Gross Error, M-estimators, Robust, Process Measurement

I. Introduction

Reliable and accurate process measurements are essential for its controlling, simulation, and management. However, measurements in mineral processing plants are always subjected to various types of errors, including random errors that are distributed independently with a mean of zero, systematic errors that occur in a non-zero mean distribution, and gross errors that are rare and do not follow a normal distribution. Gross errors are typically caused by non-random events such as leaks, measurement instantaneous deviations, and instrument failures. Consequently, measurements from an industrial circuit do not always conform to the law of mass conservation. Therefore, performance indices such as recovery are misestimated leading to bad practice of factory management. Data reconciliation is a method for correcting and optimally adjusting measured data such that the adjusted values deviate minimally from the measured data while still adhering to the law of conservation of mass and other physical constraints. The traditional approach to data reconciliation is based on the least squares error problem, which assumes no non-random errors are present (Hodouin, 2011; Mular et al., 2002; Bagajewicz, 2010). Data reconciliation is a constrained optimization problem that aims to enforce model constraints, such as mass balance, on the data to minimize the discrepancy between the estimates and measured data (Narasimhan et al., 1999; Romagnoli et al., 1999). The optimization function used is as follows (Sbárbaro et al., 2010):

$$\text{Min}\, J:\ J(X) = \sum \left(\frac{\hat{x}_i - x_i}{\sigma_i}\right)^2 \qquad (1)$$
$$Subject\ to: M\hat{x}_i = 0$$

In Eq. (1), $\hat{x}_i$ represents the matrix of the estimated values, including both the estimated values for unmeasured variables and corrected values for measured variables. x_i also represents the matrix of measured values, while σ_i denotes the standard deviation of the measured data. Variable M represents the circuit connectivity matrix that illustrates the flow of streams into the circuit (Sbárbaro et al., 2010).

The fundamental assumption of data reconciliation is that there are no systematic errors, and the lower the variance of a variable, the higher its precision, which requires less correction during the reconciliation process. However, this assumption may not hold when a variable has non-random (systematic or gross errors) (Albuquerque et al., 1996). Therefore, the correction of a stream variable is based on its variance, which indicates precision, rather than accuracy. Consequently, a stream

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containing a non-random error can propagate errors in all the other streams, and the reconciled data may be worse than the measured data and deviate further from the true values. Hence, robust data reconciliation is necessary in such cases (da Cunha et al., 2021). Robust estimation uses a specialized objective function (other than the sum of the squares of errors) for minimization. Owing to its mathematical nature, this objective function is less sensitive to deviations from ideal assumptions regarding errors, particularly outlying data. An important type of robust estimator is the maximum likelihood estimator (Llanos et al., 2015). For example, a function used for data reconciliation operations using robust methods is as follows (Jin et al., 2012):

$$\text{Min} \sum_{i=0}^{n} \rho\left(\frac{\hat{x}_i - x_i}{\sigma_i}, u\right) = \sum_{i=0}^{n} \rho(r_i, u) \quad (2)$$

Subject to: $F(x, u) = 0$

Vector r_i represents the residual of the measured variable x_i, whereas u contains the parameter estimates. The model constraints for data reconciliation during steady-state conditions are expressed through the functions F. The estimator ρ belongs to a series of robust estimators whose performance in detecting gross errors has been reported in numerous articles, such as the Kong robust estimator (Mingfang et al., 2000), weighted least-squares robust estimator (Zhang et al., 2010; Korpela, 2016; Dennis et al., 1978), and correlation estimator (Llanos et al., 2015). The Huber estimator is also important as it combines least-squares and minimum absolute deviation methods to provide a robust data estimate by reducing the bias resulting from gross errors (da Cunha et al., 2021; Huber 1992). Another robust estimator is the Cauchy estimator, which belongs to the class of probability density functions known as the Cauchy-Lorentzian distributions. The Cauchy function is often used in robust statistics and gross error detection, owing to its sensitivity to gross error values (Zhang et al., 2015; Lingke, 2006; Rey, 2012; Özyurt et al., 2004; Prata et al., 2010). Jin et al. (2012) introduced the following function for robust estimator ρ of Eq. (2):

$$\rho(r) = \begin{cases} \frac{c^2}{6}\left(1 - \left(1 - a\frac{r^2}{c^2}\right)^3\right) & if|r| \leq c \\ A\, ln\frac{r^2}{c^2} + B & if|r| \geq c \end{cases} \quad (3)$$

Where A and B are defined as follows:

$$A = \frac{(c^2 a(1-a)^2)}{2} \quad (4)$$

$$B = \frac{\left(c^2(1-(1-a)^3)\right)}{6} \quad (5)$$

In these equations, a is a tuning constant with a value ranging from 0 to 1, and c is a critical value between 1.645 and 3.090. If $|r| \leq c$, there is no gross error in the measurement. However, $|r| \geq c$ indicates the presence of at least one gross error.

Although different robust estimators are introduced in the literature, their comparison to conventional least square objective function has never been reported on a real dataset, as such dataset didn't exist. In this paper, for the first time to the authors' knowledge, such dataset is simulated and the comparison become possible. Besides, a minor modification to one of the robust estimators is implemented to enhance its ability to overcome the non-random error.

The influence function is often utilized to evaluate the impact of M estimators. By comparing the Huber, Cauchy, and Jin influence functions, it was determined that the effect of gross errors diminishes for the Cauchy estimator, showing a gradual decrease in the penetration of the influence function in the region of relative errors greater than 1.75. The effect of gross errors remains constant for the Huber estimator, with the value of the influence function unchanged in the region of relative errors greater than 0.1. As for the Jin estimator's influence function, as the relative residual increases, the calculated value of the influence function initially rises, then decreases. When the relative residual is greater than 0.3, the value of the influence function approaches zero. Therefore, the effect of gross errors can be more effectively mitigated compared to the Huber and Cauchy estimators. Thus, the Jin objective function exhibits greater robustness than the Huber and Cauchy functions (Jin et al., 2012).

II. RESEARCH METHODOLOGY

One of the significant challenges in investigating various data reconciliation methods is that the estimated data are compared to the measured data, which are prone to errors, especially in the presence of non-random errors, making this comparison unreliable. Data reconciliation could only be realy validated when real data are available. However, if real data are available, data reconciliation will be unnecessary. This contradiction makes it practically impossible to validate the results of the data reconciliation. To address this contradiction, this study suggests using artificial data. Artificial data were created by introducing disturbances into hypothetical true balanced data, transforming them into imbalanced real data with random errors, on which reconciliation is done. Thus, by having true primary balanced data, data reconciliation methods can be validated.

In this study, a hypothetical circuit with four nodes and seven streams was used to generate artificial data for the flow rates and grades, which were considered to be "true values", as shown in Table 1 (unattainable in reality). Such a circuit could refer to a mixer, crusher, classifier 1, and classifier 2. Additionally, to obtain artificially disturbed data (used as measured unbalanced data), relative variances of 12% for flows and 15% for grades were assumed, based on the assumption that repeated sampling in a large number of samples would result in such variances. Relative variance is a statistical concept denoting the variation of a variable relative to its mean. It is often expressed as a percentage, indicating the variability of the variable around its mean. The absolute variance for each data point was calculated based on these relative variances and presented in Table 1.

$$CV_x = \frac{SD_x}{\bar{X}} \tag{6}$$

Where, CV_x represents the relative variance of variable X, SD_x represents the standard deviation of variable X, $\bar{X}$ represents the mean of variable X.

To make the data more realistic, white noise was added to perfectly balanced data, using the true value as mean and the variance of the true value as the required variance for generating a random number. Generation of such noisy data were done 100 times for each point and the average and standard deviation of these 100 vlaues were obtained. The average value was assumed as the measured value for that point with known standard deviation obtained from the repetition. Thus, generated data represented "real values" measured in the plant circuit, which are unbalanced (Table 2). Data reconciliation studies were conducted on these data using both the conventional and the robust method of Jin, with the objective function of Equations 3–5, in different scenarios with or without gross errors. The study revealed that using a power of two for r in equations 3 to 5 yielded better results than using a power of one; therefore, the objective function was modified accordingly. Coding of the objective function and constraint function, as well as constrained optimization, was performed using MATLAB software.

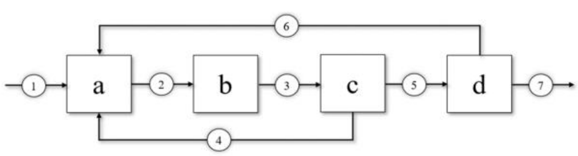

Fig. 1. Hypothetical flowsheet

For this circuit, a connectivity matrix has been prepared. In this matrix, corresponding to the nodes and streams of the circuit, there are rows and columns, respectively, and the elements of this matrix are 0, 1, and -1. In each row, corresponding to a node, the streams entering the node are indicated by 1, those exiting the node by -1, and those not connected to the node by 0. The connectivity matrix for the assumed circuit (Fig. 1) is as follows:

$$M = \begin{bmatrix} 1 & -1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & -1 \end{bmatrix}$$

Table 1. Artificially Generated Data Before Introducing Noise and Their Absolute Variances

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7
Flowrate (t/h)	109	144	144	15	129	20	109
Absolute variance of Flowrate	13.08	17.28	17.28	1.8	15.48	2.4	13.08
Grade (g/t)	21	24.84	24.84	47.69	22.18	28.61	21
Absolute variance of grade	3.15	3.73	3.73	7.15	3.33	4.29	3.15

Table 2. Artificially Generated Data after Introducing Noise (Representation of Measured Data)

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7
Flowrate (t/h)	108.19	147.31	151.34	15.59	118.51	20.38	110.96
Standard Deviation of flow rate	12.84	18.11	13.78	1.37	14.68	1.95	13.90
Grade (g/t)	21.55	25.97	26.68	49.29	21.57	28.08	20.644
Standard Deviation of grade	2.33	4.06	3.94	7.78	2.72	3.57	2.62

III. RESULTS AND DISCUSSION

A. *DATA RECONCILIATION OF A BILINEAR PROCESS USING THE CONVENTIONAL METHOD IN THE ABSENCE OF GROSS ERRORS*

The information regarding the outcomes of the data reconciliation process for the bilinear flotation procedure is presented in Table 3. This table illustrates the discrepancies between the original balanced data (which represents the true values of the variables) and the reconciled values. The final column indicates the sum of the absolute differences between the measured or reconciled data and the true values. A smaller value in this column indicates that the data are closer to the true values. The decrease in the percentage of error for the reconciled data as compared to the measured data demonstrates the ability of the data reconciliation method to approach the true values of the variables starting from the measured data. As demonstrated in Table 3, the highest error percentage is related to the flow rate and grade of stream 4, which is a recirculation stream. Overall, the error rate in all estimates was relatively low, and in this case, the reconciliation process using the least-squares method reduced the sum of absolute errors from 23.87% to 14.94% in the flow rate and from 24.25% to 13.70% in the grade. This decrease in deviation from the true data occurrs simultaneously with adhesion to mass conservation constyraints.

Table 3. Comparison of the deviation between measured and reconciled data from the true values in conventional reconciliation in the absence of gross error

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Total percentage error
True flowrate (t/h)	109	144	144	15	129	20	109	
Reconciled flowrate (t/h)	108.44	145.24	145.24	16.7	128.54	20.1	108.44	
Percentage error of the reconciled flowrate compared to the true flowrate (%)	0.51	0.86	0.86	11.33	0.36	0.50	0.51	14.94
Measured flowrate (t/h)	108.19	147.31	151.34	15.59	118.51	20.38	110.96	
Percentage error of measured flowrate relative to the true flowrate (%)	0.75	2.30	5.10	3.91	8.13	1.88	1.80	23.87
True grade (g/t)	21	24.84	24.84	47.69	22.18	28.61	21	
Reconciled grade (g/t)	21.237	25.463	25.463	49.678	22.317	28.141	21.237	
Percentage error of the reconciled grade compared to the true grade (%)	1.13	2.51	2.51	4.17	0.62	1.64	1.13	13.70
Measured grade (g/t)	21.55	25.97	26.68	49.29	21.57	28.08	20.64	
Percentage error of measured grade relative to the true grade (%)	2.62	4.55	7.41	3.35	2.76	1.86	1.69	24.25

B. DATA RECONCILIATION OF A BILINEAR PROCESS USING THE ROBUST METHOD IN THE ABSENCE OF GROSS ERRORS

Table 4 shows the outcomes of the data reconciliation process for a bilinear system using Xie's robust approach in the absence of a gross errors and when measurements were available from all flowrates and grades. The results revealed that the percentage of difference in the reconciled flow rates compared to the true flow rates in all streams was less than 5% and was almost negligible. Moreover, the total percentage of difference in the reconciled flow rates compared with the true flow rates (8.73%) was significantly lower than the total percentage of difference in reconciled flow rates compared with the true flow rates (14.94%) in the conventional method, indicating the higher accuracy of the robust method in data reconciliation, even in the absence of gross errors. By examining the plots in Fig.s 2 and 3, which illustrate the reconciled data using the robust Xie method and the conventional method, as well as the true flow rates and reconciled flowrates, it can be observed that even in situations without gross errors, the least-squares method is not optimal. The maximum likelihood method (used in the robust method) can provide a closer approximation to the true data.

Table 4. Comparison of the discrepancy between measured and reconciled data from the true values in robust reconciliation in the absence of gross error

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Total percentage error
True flowrate (t/h)	109	144	144	15	129	20	109	
Reconciled flowrate (t/h)	108.54	144.66	144.66	15.77	128.89	20.35	108.54	
Percentage error of the reconciled flowrate compared to the true flowrate (%)	0.42	0.46	0.46	5.13	0.09	1.75	0.42	8.73
Measured flowrate (t/h)	108.19	147.31	151.34	15.59	118.51	20.38	110.96	
Percentage error of measured flowrate relative to the true flowrate (%)	0.75	2.30	5.10	3.91	8.13	1.88	1.80	23.87
True grade (g/t)	21	24.84	24.84	47.69	22.18	28.61	21	
Reconciled grade (g/t)	21.191	25.31	25.31	50.049	22.283	28.107	21.191	
Percentage error of the reconciled grade compared to the true grade (%)	0.91	1.89	1.89	4.95	0.46	1.76	0.91	12.77
Measured grade (g/t)	21.55	25.97	26.68	49.29	21.57	28.08	20.64	
Percentage error of measured grade relative to the true grade (%)	2.62	4.55	7.41	3.35	2.76	1.86	1.69	24.25

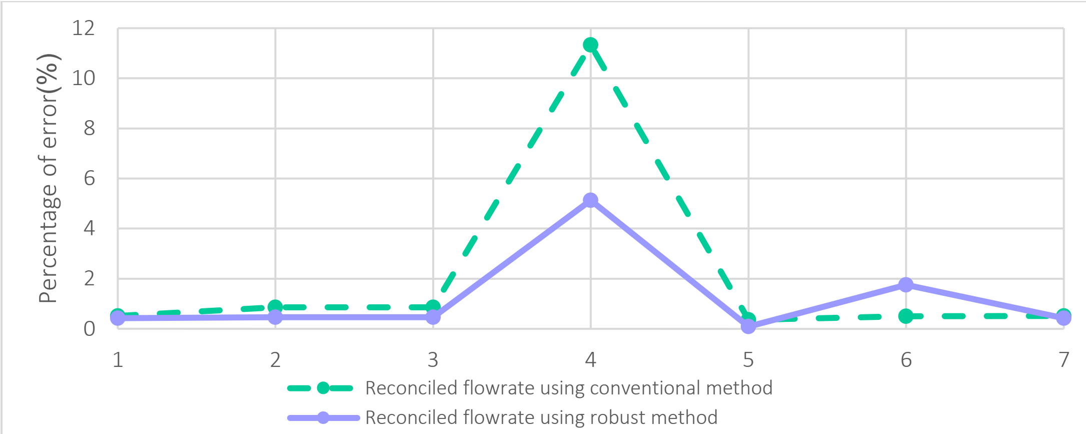

Fig 2. Comparison of the discrepancies in reconciled flowrates compared to true flowrates using conventional and robust reconciliation methods

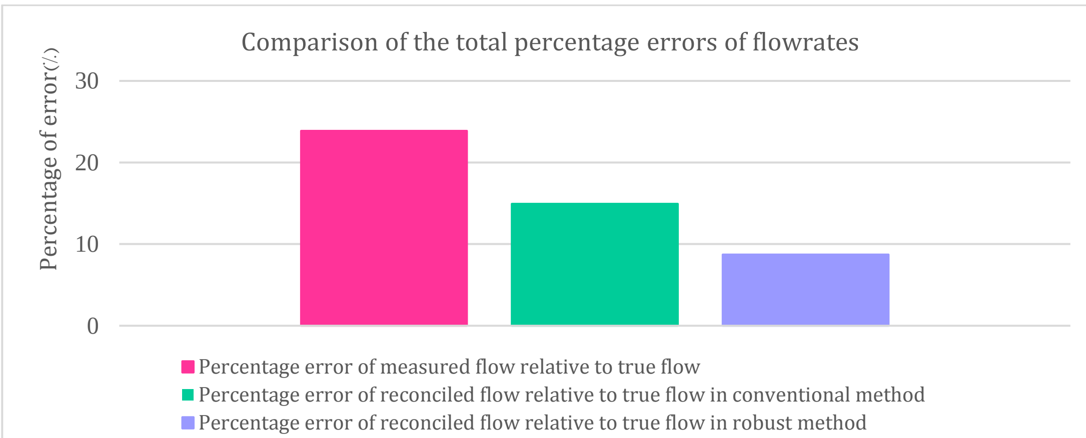

Fig 3. Comparison of the total percentage of errors of measured, conventionally reconciled, and robustly roconciled flowrates relative to true flowrates

C. DATA RECONCILIATION OF A BILINEAR PROCESS USING THE CONVENTIONAL METHOD IN THE PRESENCE OF GROSS ERROR IN ONE STREAM

The results displayed in Table 5 show the inefficiency of the conventional reconciliation method in compensating the gross error in stream 4. The percentage error of the measured data compared with the true data of Stream 4 in the presence of gross error was 100%, which decreased slightly to approximately 95% in the reconciled data. However, this gross error also affects the estimation of reconciled values for other streams, leading to a total sum of absolute errors in the streams reaching 124.66%, which exceeds the sum of the errors of the measured data. These findings indicate that the conventional method was not successful in correcting the gross error, and that in the presence of a gross error, reconciled values might be worse than measured data in terms of distance from the true values.

D. DATA RECONCILIATION OF A BILINEAR PROCESS USING THE ROBUST XIE METHOD IN THE PRESENCE OF GROSS ERROR IN STREAM 4

After conducting data reconciliation of a bilinear process in the presence of a gross error in recirculation stream 4 using the robust Xie method, the following outcomes were obtained. Results of the reconciliation process using the conventional and robust Xie methods were compared to the true flow rates in Fig. 4, indicating that the robust method was effectively performed the reconciliation process. Table 6 displays a comparison of the measurement errors using the robust Xie method in the presence of a gross error in recirculation stream number 4, including the percentage error of the reconciled data compared to the true data, and the percentage error of measured data compared to the true data. The results showed that the percentage error for all streams and grades was generally very low, with reasonable error percentages for all cells.

Table 5. Comparison of the discrepancy between measured and reconciled data with true data in conventional reconciliation method under a gross error in stream number 4.

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Total percentage error
True flowrate (t/h)	109	144	144	15	129	20	109	
Reconciled flowrate (t/h)	104.78	152.83	152.83	29.21	123.62	18.85	104.78	
Percentage error of the reconciled flowrate compared to the true flowrate (%)	3.87	6.13	6.13	94.73	4.17	5.75	3.87	124.66
Measured flowrate (t/h)	108.19	147.31	151.34	30.00	118.51	20.38	110.96	
Percentage error of measured flowrate relative to the true flowrate (%)	0.75	2.30	5.10	100.00	8.13	1.88	1.80	119.96
True grade (g/t)	21	24.84	24.84	47.69	22.18	28.61	21	
Reconciled grade (g/t)	20.74	26.99	26.99	48.8	21.83	27.88	20.74	
Percentage error of the reconciled grade compared to the true grade (%)	1.24	8.66	8.66	2.33	1.58	2.55	1.24	24.26
Measured grade (g/t)	21.55	25.97	26.68	49.29	21.57	28.08	20.64	
Percentage error of measured grade relative to the true grade (%)	2.62	4.55	7.41	3.35	2.76	1.86	1.69	24.25

Table 6. Comparison of the discrepancy between measured and adjusted data with true data in robust reconciliation method under a gross error in stream number 4.

Variable	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5	Stream 6	Stream 7	Total percentage error
True flowrate (t/h)	109	144	144	15	129	20	109	
Reconciled flowrate (t/h)	109.86	147.99	147.99	16.38	131.61	21.75	109.86	
Percentage error of the reconciled flowrate compared to the true flowrate (%)	0.79	2.77	2.77	9.20	2.02	8.75	0.79	27.09
Measured flowrate (t/h)	108.19	147.31	151.34	30.00	118.51	20.38	110.96	
Percentage error of measured flowrate relative to the true flowrate (%)	0.75	2.30	5.10	100.00	8.13	1.88	1.80	119.96
True grade (g/t)	21	24.84	24.84	47.69	22.18	28.61	21	
Reconciled grade (g/t)	21.16	25.38	25.38	50.09	22.31	28.09	21.16	
Percentage error of the reconciled grade compared to the true grade (%)	0.76	2.17	2.17	5.03	0.59	1.82	0.76	13.31
Measured grade (g/t)	21.55	25.97	26.68	49.29	21.57	28.08	20.64	
Percentage error of measured grade relative to the true grade (%)	2.62	4.55	7.41	3.35	2.76	1.86	1.69	24.25

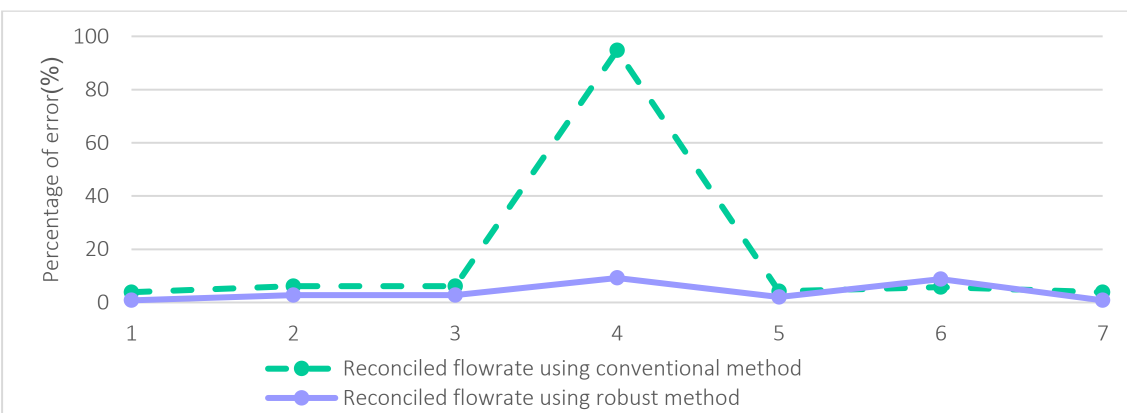

Fig. 4. Comparison of the discrepancies in reconciled flowrates compared to true flowrates using conventional and robust reconciliation methods in the presence of a gross error in stream number 4

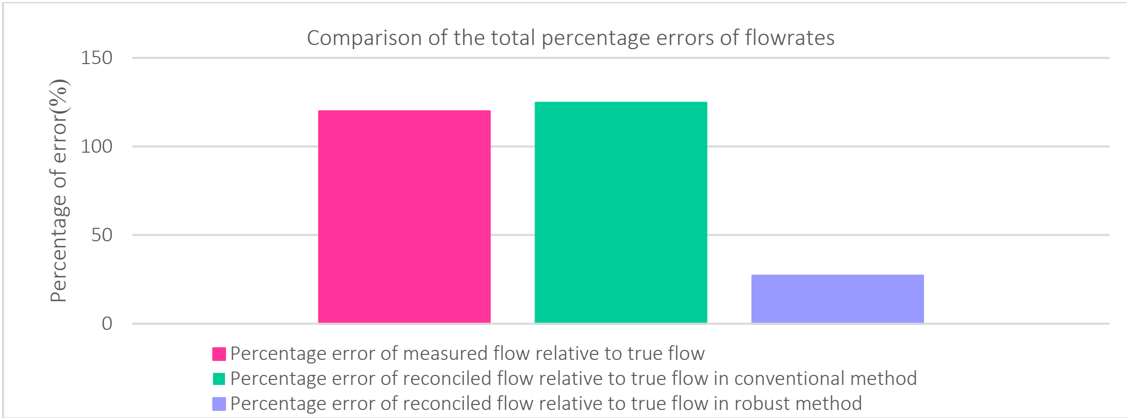

Fig. 5. Comparison of the total percentage of errors of measured, conventionally reconciled, and robustly rocnciled flowrates relative to true flowrates in the presence of a gross error in stream number 4

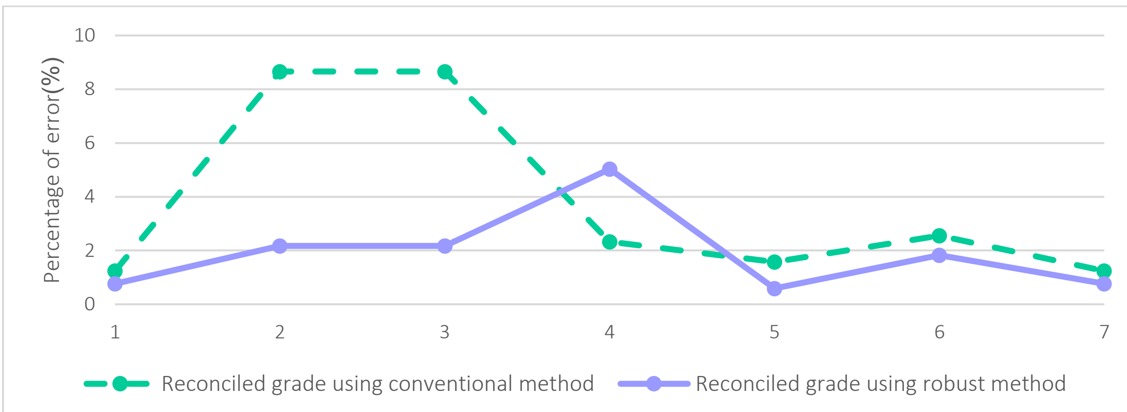

Fig. 6. Comparison of the discrepancies in reconciled flowrates compared to true grades using conventional and robust reconciliation methods in the presence of a gross error in stream number 4

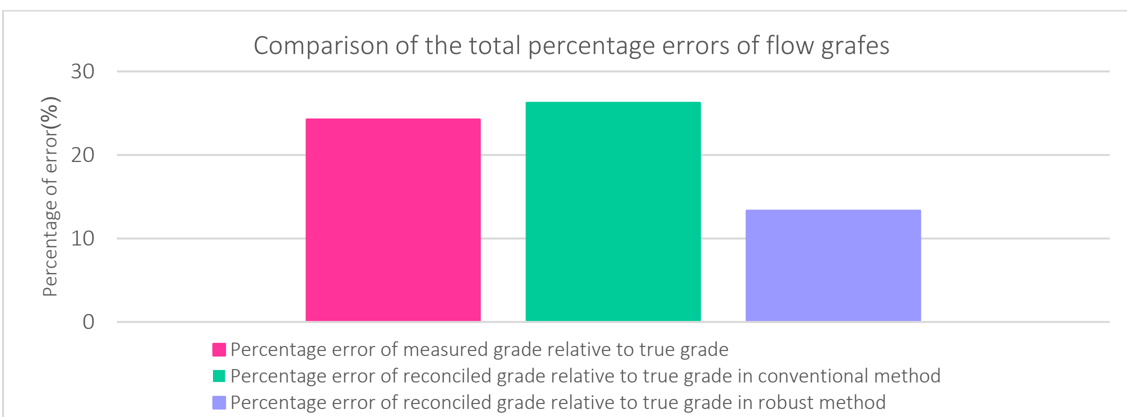

Fig. 7. Comparison of the total percentage of errors of measured, conventionally reconciled, and robustly roconciled grades relative to true grades in the presence of a gross error in stream number 4

In stream number 4, where a gross error exists, the percentage error of the reconciled flow rate compared with the true flow rate is significantly lower than that of the measured flow rate compared with the true flow rate of conventional reconciliation method. This highlights the high capability of the robust method to handle outliers and erroneous data. The total percentage error for the reconciled flow rate compared to the true data was very low (27%), whereas the total percentage error of the measured flow rate compared to the true data was 119.96%, indicating a significant enhancement of roconciled values compared to measurments.

IV. CONCLUSION

To the authors' best knowledge, for the first time, results of two rconciliation methods, namely robust and conventional ones, were compared to each other, since simulated sampling data were generated from true balanced data and the trues values were available. The following comparisons highlight the results:

- The robust method, when employed under normal circumstances and in the absence of gross errors, enhances the accuracy of the flow rate and grade estimations, bringing the results closer to their true values.
- However, when a gross error exists in a stream, the conventional approach fails to correct the error and instead yields data estimates that are further from the true values. Such an error in stream 4 negatively affected the other streams, causing their estimates to diverge from the true values when using the conventional method.
- In contrast, the robust method effectively handles gross errors in a stream, leading to a significant enhancement in the accuracy of the reconciled data compared with the conventional method. This resulted in a substantial decrease in the percentage error during data reconciliation. These outcomes illustrate the exceptional ability of the robust method to handle outliers and erroneous data.

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