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Integrating data reconciliation into material flow cost accounting: The case of a petrochemical wastewater treatment plant

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ABSTRACT

Material flow cost accounting analyzes input/output relations of material flows in the production process based on mass balance principles. However, the measured data of a process contains errors representing a mass imbalance in the system such as that of a wastewater treatment plant. Therefore, measured data should be verified before establishing mass balance and, subsequently, material flow cost accounting. Hence, in this work, a novel practical stepwise methodology using data reconciliation technique is introduced to improve the accuracy and certainty of measurements before material flow cost accounting. A full-scale petrochemical wastewater treatment plant was selected to establish this methodology. The presented results of this case study show an error of −3.22% (−35244 t/year) between total input and output streams of wastewater treatment plant demonstrating mass imbalance in the system. However, the overall mass balance could be closed by simultaneously solving the incidence matrix (system of balances). The results revealed that by including data reconciliation into material flow cost accounting, an accurate mass balance can be performed, which is a key element in material flow cost accounting calculations. The comparison results showed a relatively significant difference between material flow cost accounting for reconciled and measured data (unreconciled). The developed approach provides a reliable set of data for implementing material flow cost accounting in the system. Therefore, using this novel stepwise approach will help decision-makers to enhance both financial and environmental performances more confidently and to define appropriate improvement plans.

1. Introduction

Increased consumption of natural resources followed by the generation of waste are inevitable consequences of rapid urbanization and industrial growth which affect both the environment and human life. To cope with this, several environmental management tools have been introduced by environmental protection agencies that require business organizations to more accurately account for the environmental impacts of their businesses (Fakoya and van der Poll, 2013). Although environmental management tools are effective in reducing adverse environmental impacts, they may impose a financial burden on the companies implementing them (Kokubu and Kitada, 2015). Material flow cost accounting (MFCA), a promising environmental management accounting (EMA) tool (Fakoya and van der Poll, 2013), can help industrial companies improve their environmental and profitability performance (Chompu-inwai et al., 2015). Unlike traditional cost accounting methods in which costs are attributed to products, MFCA analyzes the cost of products and the costs associated with material and energy losses (Guenther et al., 2015; Prox, 2015), thereby increasing the transparency in accounting for materials by highlighting the hidden costs and inefficiencies (Rieckhof et al., 2015). MFCA provides detailed information for organizations about the full costs of wastes (Fakoya and van der Poll, 2013) and opportunities for reducing materials use (Christ and Burritt, 2016). This

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advantage of MFCA compared to other classic accounting approaches can be a motivator for interested manufacturing industries to mitigate environmental impacts and improve financial performance at the same time (Kokubu and Kitada, 2015).

The original concept of MFCA was developed in Germany in the late 1990s; however, this method reached its great success in Japan in the 2000s. Up to 300 Japanese enterprises applied the MFCA approach by the year 2010 (Schmidt et al., 2015). MFCA received more attention when a norm on MFCA as ISO 14051 was published in 2011 (Christ and Burritt, 2015; ISO14051, 2011). Today, MFCA is expanding globally, and the positive outcomes of its employment are being reported. To date, MFCA has been successfully applied in various industrial companies with the aim of waste recovery (Wan et al., 2015), improving technology to increase productivity (Jakrawatana et al., 2016), enhancing the accuracy of information for the decision-making process (Chang et al., 2015), waste reduction (Kasemset et al., 2015), and optimization of corporate manufacturing processes (Kasemset et al., 2013). MFCA has also been applied in combination with the concepts of enterprise resource planning (ERP) (Fakoya and van der Poll, 2013), existing environmental management systems (EMS) (Fakoya and van der Poll, 2012), and the design of experiments (DOE) (Chompu-inwai et al., 2015) to reduce materials consumption and improve waste-reduction decisions.

To our knowledge, all MFCA studies to date in industries and processes were performed on solid material flows based on the mass balance model. In their recently published work, Mahmoudi et al. (2017) employed MFCA for efficiency improvement in the wastewater treatment plant (WWTP) of an oil refining company. Their study is the first report of employing MFCA in a system based on liquid flow streams. They performed mass balance calculations for all in- and outgoing mass flows of WWTP. Mass balance equation results were used to calculate the amount of losses, annual costs, and benefits in the treatment processes. Although the mass balance approach was applied, a technique for improving the reliability and consistency of measurements was not considered in their study. Because flow measurements are never 100% accurate due to breakdowns in the measuring devices and process dynamics (Shakerkhatibi et al., 2016), measured data balances can never be closed perfectly.

In general, MFCA is a tool which analyzes the input/output relations of material flows in the production process based on the mass balance principle (Nakajima, 2015). Generally, the measured data of a process contains two types of error: random and gross, causing mass imbalance in systems such as a WWTP (Wongrat et al., 2005). In order to establish an accurate mass balance in the system, the quality of measurements needs to be verified. Data reconciliation (DR) is a statistical technique based on mass balance calculations that is used to enhance the accuracy and certainty of data by minimizing random errors in measurements (Spindler, 2014; Zhang et al., 2014). Applying the DR technique prior to mass balance analysis will increase the reliability and accuracy of results that are used for decision-making and performance evaluation processes (Oliveira et al., 2015). The DR technique has already been successfully implemented in various systems in the fields of process engineering (Rafiee and Behrouzshad, 2016), performance evaluation (Behnami et al., 2016; Jiang et al., 2014), benchmarking, and plant modeling (Puig et al., 2008).

In this study, MFCA was established in a petrochemical WWTP to improve efficiency and visualize treatment costs and the cost of inefficiencies. For the first time, a novel practical stepwise methodology using DR technique was applied to enhance the quality of measurements intended for use in MFCA calculations. By including DR in MFCA, the reliability and accuracy of MFCA outcomes can be improved, which enables decision-makers to more accurately and confidently enhance both financial and environmental profitability.

2. Methodology

In this research, MFCA is applied in a full-scale petrochemical WWTP. Data reconciliation technique is also used to improve the quality of data in advance of establishing MFCA calculations. The concepts of MFCA and DR technique as well as the integrated approach of MFCA and DR are presented in the following sections.

2.1. Description of studied WWTP

A full-scale petrochemical WWTP located in the Tabriz petrochemical company (TPC) in northwestern Iran was selected for investigation in this study. The WWTP was designed with a capacity of 4800 m^3/day using extended aeration activated sludge system. The current operating capacity of the WWTP is 2544 m^3/day. The influent wastewater of WWTP is a mixture of effluents from various production units, saline wastewater, rainfall water, and sanitary wastewater. The WWTP is composed of primary treatment (American petroleum institute (API) oil separator, equalization, coagulation-flocculation, dissolved air flotation (DAF), and neutralization), secondary treatment (biological reactor, primary clarifier, coagulation, and secondary clarifier), and tertiary treatment (sand filtration). The final treated effluent of WWTP is used mainly for irrigation or firefighting purposes within the petrochemical complex. The process flow diagram of the studied WWTP is illustrated in Fig. 1. It is necessary to mention that the data presented in Fig. 1 represents the raw data derived from measuring the flowrate (t/year) of various streams existing in the selected WWTP.

2.2. Material flow cost accounting

As one of the most basic and effective EMA tools, MFCA helps industrial organizations establish a cleaner production approach. MFCA is a “tool for quantifying the flows and stocks of materials in processes or production lines in both physical and monetary units,” (ISO14051, 2011). Material and energy consumptions are greatly important for industrial companies regarding economy and environment; thus, EMA puts special emphasis on material flows and energy use as well as their associated costs (Christ and Burritt, 2015). Moreover, it has been proven that the costs of wasted materials comprise about 40%–70% of total costs for individual organizations (Jasch, 2009). Therefore, by analyzing the costs of wasted materials and inefficiencies, MFCA provides opportunities for companies to reduce wastage, concurrently improve environmental and economic performance, and optimize the use of various resources (Schaltegger and Zvezdov, 2015; Yagi and Kokubu, 2018).

MFCA traces all the materials entering the production process and classifies them into two categories: positive and negative products (Jasch, 2009). The desired products that can be sold are positive products, while waste and emissions are negative (undesired) products (Jakrawatana et al., 2016). Using the MFCA technique, the processes with a large amount of negative products can be identified, and solutions for improving efficiency and reducing negative products are provided (Kasemset et al., 2015).

Under MFCA calculations, the costs of manufactured products are categorized into four distinct classes: material cost, energy cost, system cost (e.g., personnel costs and depreciation), and waste management cost (e.g., cost of waste disposal and pollutants emission control) (ISO14051, 2011; Rieckhof et al., 2015).

To establish MFCA, the collected data is inputted into the MFCA calculations, and the costs of positive and negative products are allocated based on the mass balance concept. The cost of positive

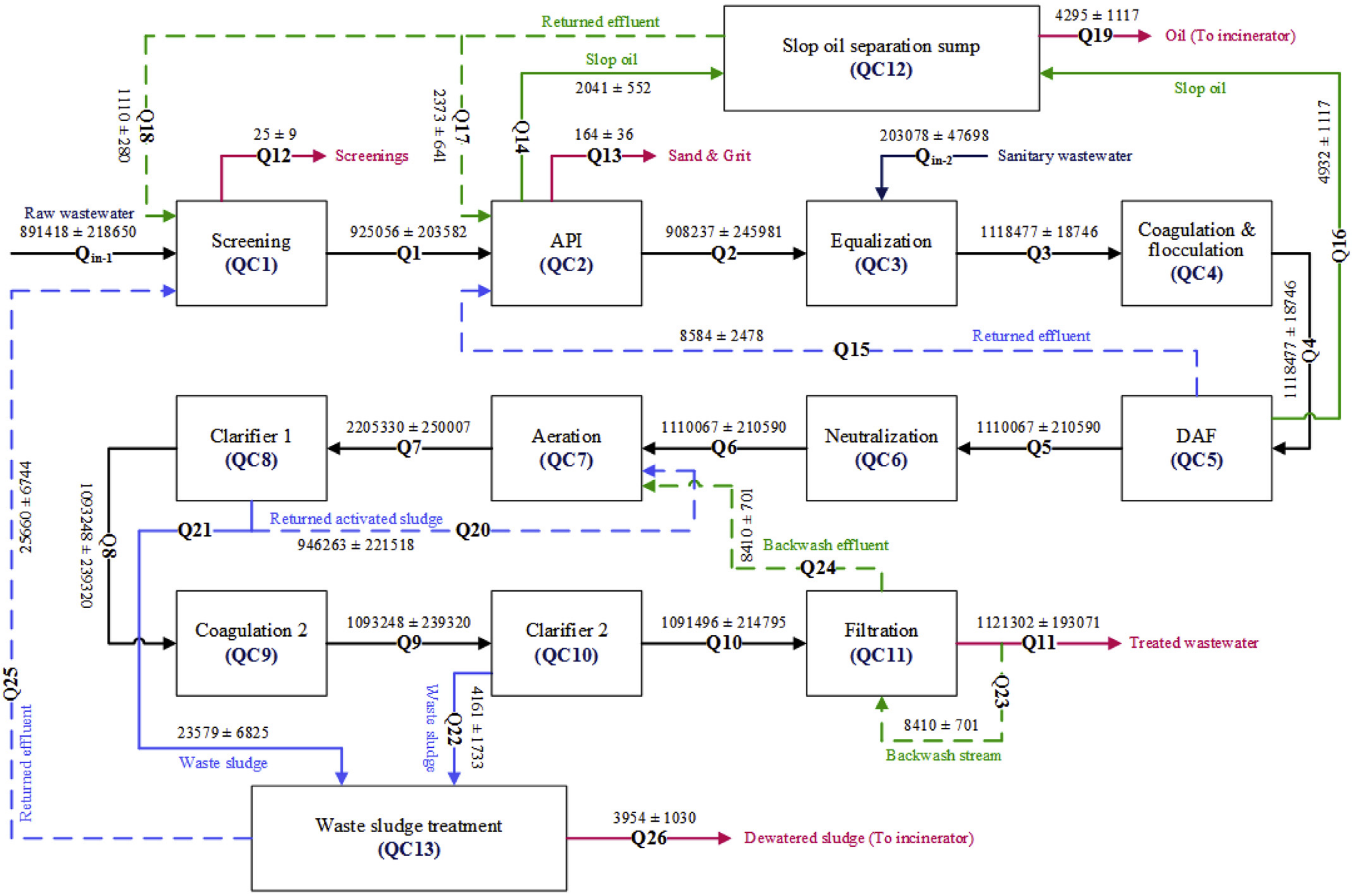

Fig. 1. Schematic flow diagram of petrochemical WWTP.

products is the cost put into the finished products of one process released to the next process, while the cost of negative products is related to wasted or recycled materials (Jakrawatana et al., 2016).

To establish a mass balance for a quantity center (QC), the following equation can be used:

$$\sum_{i=1}^{n} I_i = \sum_{j=1}^{p} P_j + \sum_{k=1}^{w} W_k \tag{1}$$

where I_i, P_j, and W_k are the mass of ith input (raw) material, jth desired product, and kth wasted material, respectively, and n, p, and w represent the total number of input materials, desired products, and wasted materials for a QC, respectively.

The total cost of process C_{pc} for a QC is composed of material costs, C_{mat}, energy costs, C_{engy}, system costs, C_{sys} and waste management cost, C_{wm} given as:

$$C_{pc} = C_{mat} + C_{engy} + C_{sys} + C_{wm} \tag{2}$$

C_{mat} represents the cost of n raw materials that is required in a process and can be calculated as follows:

$$C_{mat} = \sum_{i=1}^{n} C_{mat_i} I_i \tag{3}$$

where C_{mat_i} stands for the unit cost of raw material i. Likewise, C_{engy} can be written as:

$$C_{engy} = \sum_{e=1}^{E} C_{engy_e} E_e \tag{4}$$

where C_{engy_e} represents the unit cost of energy types e, and E_e is the amount of energy types e required in a process. System costs are taken as C_{sys} and can be defined by:

$$C_{sys} = \sum_{s=1}^{S} C_{sys_s} S_s \tag{5}$$

where C_{sys_s} refers to the unit cost of sth item including direct and indirect manpower costs, spare parts cost and depreciation cost, and S_s is the required amount of sth item involved in a process. System unit cost is calculated based on the sth items and prorated for all QCs. Waste management cost is the cost of handling and final disposal of wastes in a process and can be calculated as follows:

$$C_{wm} = \sum_{k=1}^{w} C_{wm_k} W_k \tag{6}$$

where C_{wm_k} is the unit cost for management of kth waste materials (screenings, sand and grit, slop oil and biological sludge).

2.3. Data reconciliation

Process measurements are inevitably accompanied by two types of errors: gross errors (such as malfunctioning instruments, measurement biases, and process leaks) and random errors, leading to inconsistencies in energy and material balances (Romagnoli and Sanchez, 1999) and inferior performance of a process (Chattinnawat and Bilen, 2017). It is necessary to reduce these errors and adjust the measurements in order to obtain reliable and accurate sets of process data for use in process control and optimization purposes (Crowe, 1996). Data reconciliation (DR) is a mathematical filtering technique that is used to adjust or reconcile the process measurements by reducing the influence of random errors based on the concept of redundancy between the process model and the measurements model (Yélamos et al., 2007). Thereupon, the reconciled process data conforms to the conservation laws and other constraints and enables energy and mass balance to close (Crowe, 1996).

In the absence of gross errors, the measurements can be mathematically written as follows (Lim et al., 2012; Narasimhan and Bhatt, 2015):

$$y = x + \varepsilon \tag{7}$$

where y is the measurement vector, x is the vector of true values of variables, and ε stands for unknown random error in measurement. It is assumed that the expected value of random error (ε) is the null vector, i.e., $E(\varepsilon) = 0$, and its variance is as follows:

$$var(\varepsilon) = E[\varepsilon^2] = \sigma^2 \tag{8}$$

where σ indicates the standard deviation of the measurement error.

The DR technique provides reconciled data by minimizing the sum of the squares of errors between measurements and model values, subject to a number of constraints:

$$MIN\ (y-x)^T\psi^{-1}(y-x) \tag{9}$$

Subject to $A\ (y - \varepsilon) = 0$.where ψ is the covariance matrix of measurement errors describing the measurement uncertainties, and A is the submatrix corresponding to measured variables for linear models (which is the balance equation). In order to establish the incidence matrix, each QC (or subsystem compartments) in the WWTP has been considered as a node, and a matrix has been prepared based on the available data to make mass balances around each QC (node). In the incidence matrix (A), each row represents a node, and each column represents a flow stream. Each element in A is either +1, −1 or 0, depending on whether the corresponding flow is an input stream, an output stream, or not associated with this node.

For implementing a data reconciliation technique in a system such as that of a WWTP, the uncertainty of the measurements needs to be evaluated (BIPM et al., 2008). The standard deviation was used as a measure of the uncertainty of the measurements. In this work, we assumed that the error of the measured data follows a normal distribution, which is the usual assumption in data reconciliation calculations (Narasimhan and Jordache, 1999).

A constrained optimization problem can be solved analytically by including Lagrange multipliers (λ) in the solution (Crowe et al., 1983; Narasimhan and Jordache, 1999):

$$L(y,\lambda) = (y-x)^T\psi^{-1}(y-x) - 2\lambda^T Ax \tag{10}$$

Substituting Eq. (7) in Eq. (10) yields:

$$L(y,\lambda) = \varepsilon^T\psi^{-1}\varepsilon - 2\lambda^T(Ay - A\varepsilon) \tag{11}$$

Since ψ is the positive definite covariance matrix and the constraints are linear, the following equations are obtained after differentiating Eq. (10) with respect to ε and λ and equating them to zero:

$$\frac{\partial L}{\partial \varepsilon} = 2\psi^{-1}\varepsilon + 2A^T\lambda = 0 \tag{12}$$

$$\frac{\partial L}{\partial \lambda} = A(y-\varepsilon) = 0 \tag{13}$$

Thus, the values of ε and λ can be obtained through:

$$\varepsilon = -\psi A^T\lambda \tag{14}$$

$$\lambda = -(\psi A^T)^{-1}\varepsilon \tag{15}$$

Multiplying and dividing with A on the right-hand side of Eq. (15) gives:

$$\lambda = -A^{-1}(\psi A^T)^{-1}A\varepsilon \tag{16}$$

Eq. (16) can be simplified as follows:

$$\lambda = -(A\psi A^T)^{-1}A\varepsilon \tag{17}$$

Rearranging Eq. (13) yields:

$$A\varepsilon = Ay \tag{18}$$

Substituting Eq. (18) in Eq. (17) yields:

$$\lambda = -(A\psi A^T)^{-1}Ay \tag{19}$$

Substituting Eq. (19) in Eq. (14) yields:

$$\varepsilon = \psi A^T(A\psi A^T)^{-1}Ay \tag{20}$$

By substituting Eq. (20) in Eq. (7), the estimate of the process variable can be calculated:

$$y_{estimated} = y - \varepsilon = y - \psi A^T(A\psi A^T)^{-1}Ay \tag{21}$$

This method has been implemented in MATLAB program and applied on measured flow rates.

2.4. Implementing DR and MFCA in WWTP

The following steps give the procedure for implementing DR and MFCA in a WWTP:

Step 1: Definition of the system boundaries. This step is widely accepted in implementing MFCA in a system (Christ and Burritt, 2015). It is achieved through studying the plant and its processes to develop a basic understanding of the materials and flows.
Step 2: Determination of appropriate QCs. A QC is a part of the process for which inputs and outputs are quantified in physical and monetary units (ISO14051, 2011).
Step 3: Collection of required data. In this step, all inputs and outputs against each QC as well as material losses and waste quantities are quantified.
Step 4: Implementation of the DR technique. Within this step, all measured flows are reconciled, and errors are identified (as mentioned in Sec. 2.3) to perform closed material flow balance.
Step 5: Assignment of monetary values for inputs and outputs of each QC within the MFCA boundary. In this step, MFCA calculations can be done based on reconciled data.

Step 6: Providing possible and applicable solutions for waste minimization, increasing the efficiency of various processes and decreasing the overall costs of the treatment system.

For ease of understanding, the step-by-step framework used in this study is shown in Fig. 2.

3. Results and discussion

The results obtained from the implementation of the integrated approach of MFCA and DR techniques are presented in the following sections.

3.1. Application of proposed method

In this section, the method illustrated in Fig. 2 is explained step-by-step in a case study.

3.1.1. Determination of QCs

In the investigated WWTP, each treatment unit was considered as a QC, and all input and output streams were identified. In a related study on implementing MFCA in WWTP conducted by Mahmoudi et al. (2017), only three QCs were defined, including physical treatment, biological treatment, and chemical treatment. More precisely, various processes of WWTP can be considered as QCs to clearly identify the inputs and outputs and establish an accurate mass balance. Accordingly, the following 13 QCs were determined in this study (Fig. 1): screening API, equalization, coagulation-flocculation, DAF, neutralization, aeration, primary clarifier, secondary coagulation, secondary clarifier, filtration, slop oil separation sump, and waste sludge treatment. Although no significant change was observed in the inlet and outlet flows of some treatment units (e.g., primary coagulation and flocculation, neutralization and secondary coagulation), these units were also considered as QC, because chemicals and energy (electricity) were used in these units and affected the treatment cost calculations.

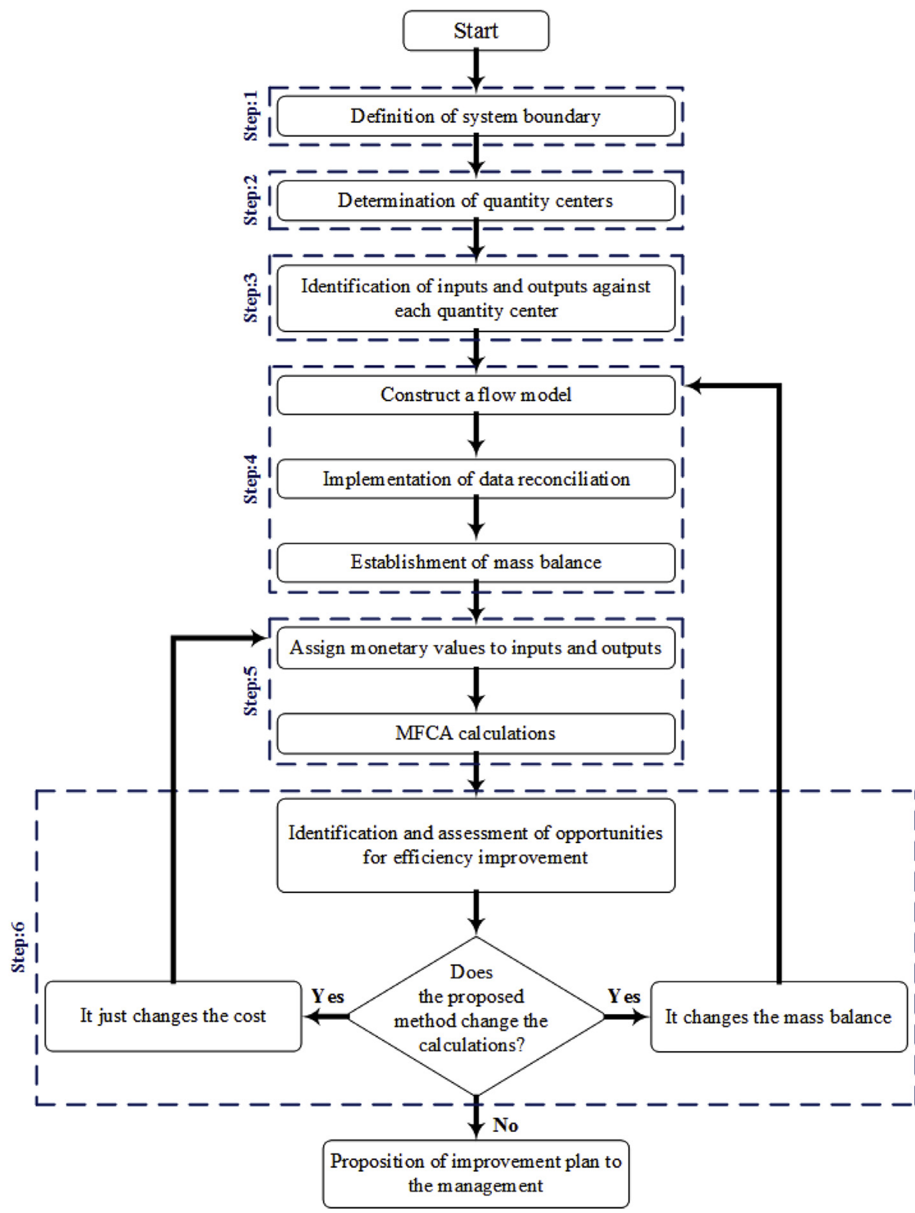

Fig. 2. Step-by-step methodology for MFCA and DR implementation in a WWTP.

3.1.2. Flow measurements

The overall in- and outgoing flow measurements were done and introduced in a matrix, as presented in Table 1, to perform overall mass balance in the system. The incidence matrix resulting from the plant layout (Table 1) demonstrates how each compartment (QC) is affected by different streams and how they interact. As can be seen in Table 1, the total measured flow rate of the inlet and the outlet streams against each QC is a figure other than zero, indicating that the mass balance cannot be closed. These errors in measured values frequently happen in practice, particularly in full-scale wastewater treatment systems, because of the breakdown of the flow measuring devices, sampling conditions, analytical procedures, and so on (Doherty et al., 2017; Rieger et al., 2010). Obviously, neglecting these errors leads to mass imbalance and, consequently, erroneous MFCA calculations. Likewise, high standard deviation values were observed in the measured data, demonstrating the high variability of measurements which is due to the influent flow dynamics (Puig et al., 2008). As already mentioned in the introduction, the reliability of the MFCA results depends on establishing an accurate mass balance in the system. Therefore, the DR technique, a powerful tool for detecting random errors and improving the general data quality, is needed to adjust the stream flow rates and enable the balance to close (Martins et al., 2010).

3.1.3. Data reconciliation and mass balance results

The DR technique employs the incidence matrix to calculate one solution and, concurrently, reduces the inaccuracy and uncertainty of the measurements. The results of overall mass balance before and after balancing and their corresponding relative standard deviations (RSD) are shown in Table 2, together with the estimated error between the measured data and the balanced data. The total mass balance based on the measured data presented an estimated imbalance of −3.22% (−35244 t/year) between total input and output streams of WWTP, making it almost impossible to use the unbalanced data in MFCA calculations. Based on the results shown in Table 2, it is observed that after simultaneously solving the incidence matrix (Table 1), the error of reconciled data is equal to zero; therefore, the mass balance could be closed.

The results also demonstrate that the standard deviation and relative error of measurements were drastically improved by using the DR technique, particularly for the raw and treated wastewater. Fig. 3 shows the calculation of mass balance in each QC based on the reconciled data. As can be seen, the mass balance for each QC is closed, and total inputs and outputs against each QC is equal to zero. It needs to mention that the studied WWTP is a continuous treatment system; therefore, remaining or changing stocks within QCs cannot be occurred. The establishment of an accurate mass balance in a system is essential for performing more precise MFCA calculations. In this way, decision-makers will be able to define the improvement plans more confidently.

3.1.4. MFCA calculations

In this case study, it was assumed that the influent wastewaters, including Q_{in-1} and Q_{in-2}, have zero cost because the process wastewater is collected from various petrochemical units; thus, it is practically impossible to allocate a cost on influent wastewater. Moreover, the cost of influent wastewater has no effect on the MFCA calculations, because the purpose is to calculate the total cost of the plant and the cost associated with each treatment unit. Therefore, in this study, the influent streams, including Q_{in-1} and Q_{in-2}, were considered to have zero cost, and their actual costs are increased while passing through the different QCs. Finally, the total costs of wastewater treatment, as well as the costs associated with the waste streams are calculated. It should also be noted that there are some returning flows, including Q_{15}, Q_{17}, Q_{18}, Q_{20}, Q_{23}, Q_{24} and

Table 1
Error diagnosis of the flow measurements.

Stream (t/year)	Compartment												
	QC1	QC2	QC3	QC4	QC5	QC6	QC7	QC8	QC9	QC10	QC11	QC12	QC13
Q_{in-1}	891418												
Q_{in-2}			203078										
Q_1	−925056	925056											
Q_2		−908237	908237										
Q_3			−1118477	1118477									
Q_4				−1118477	1118477								
Q_5					−1110067	1110067							
Q_6						−1110067	1110067						
Q_7							−2205330	2205330					
Q_8								−1093248	1093248				
Q_9									−1093248	1093248			
Q_{10}										−1091496	1091496		
Q_{11}											−1121302		
Q_{12}	−25												
Q_{13}		−164											
Q_{14}		−2041										2041	
Q_{15}		8584			−8584								
Q_{16}					−4932							4932	
Q_{17}		2373										−2373	
Q_{18}	1110											−1110	
Q_{19}												−4295	
Q_{20}							946263	−946263					
Q_{21}								−23579					23579
Q_{22}										−4161			4161
Q_{23}											8410		
Q_{24}							8410				−8410		
Q_{25}	25660												−25660
Q_{26}													−3954
Errors	**−6893**	**25571**	**−7162**	**0**	**−5106**	**0**	**−140590**	**142240**	**0**	**−2409**	**−29806**	**−805**	**−1874**

Elements with negative sign are outflow streams, and positive elements are inflow streams.

Table 2
Overall mass balance calculations (Annual basis).

Flow (t/year)	Measured data		Balanced data		Estimated error (%)
	Average ± SD	RSD (%)	Average ± SD	RSD (%)	
Influent flow					
Process wastewater	891418 ± 218650	24.5	917207 ± 79190	8.6	2.8
Sanitary wastewater	203078 ± 47698	23.5	196542 ± 44150	22.5	−3.3
Effluent flow					
Treated effluent	1121302 ± 193071	17.2	1106927 ± 71832	6.5	−1.3
Sand & Grit	164 ± 36	21.9	156 ± 11	7.1	−5.1
Screenings	25 ± 9	36.0	23 ± 4	17.4	−8.7
Slop oil	4295 ± 1117	26.0	3238 ± 544	16.8	−32.6
Waste sludge	3954 ± 1030	26.1	3405 ± 441	13.0	−16.1
Error in measurements	−35244		0		

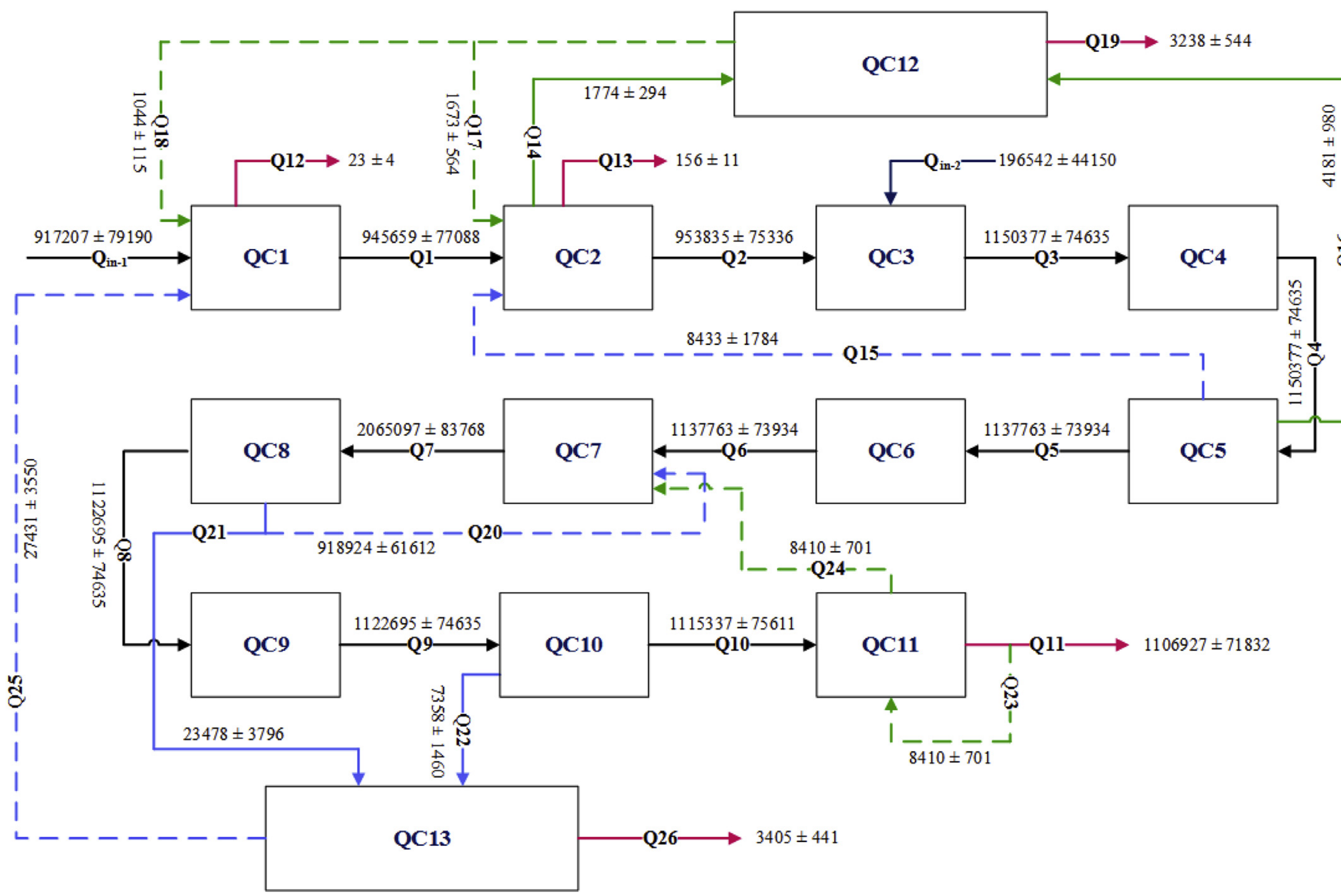

Fig. 3. Mass flow diagram of petrochemical WWTP based on the reconciled data (t/year).

Q_{25}, in the WWTP (Fig. 3), and their associated costs can be calculated in the first cycle of cost allocation. Subsequently, the calculated cost of return flows is used in the second cycle of cost allocation to compute the actual cost of each QC and the final treatment cost (assuming that each returning flow is cycled only once in the system).

From Fig. 1, it can be seen that there are two types of products in the studied WWTP: (1) treated effluent of each QC as a positive product, and (2) screenings, sand and grit, slop oil, and dewatered sludge as negative wastes. The final effluent of WWTP (filtration outlet) is currently used for irrigation or firefighting purposes within the petrochemical complex.

To perform complete MFCA calculations, determining the energy, system, and material costs for each QC is required in order to estimate the final value of the influent stream. It is necessary to mention that such costs as direct and indirect manpower costs, depreciation costs, spare parts costs, etc. were included in system costs and prorated for all QCs. Waste management costs were included in the present study because the petrochemical company spends a considerable amount for waste treatment.

The material flow cost accounting of the WWTP based on reconciled data is shown in Fig. 4. As can be seen, the main material (influent wastewater) is first inputted to the WWTP with zero cost; after that, its cost increases during the treatment steps. Considering the data presented in Fig. 4, 1113749 t/year of materials ($Q_{in-1} + Q_{in-2}$) entered the treatment plant; the amount of materials leaving the WWTP as positive products was 1106927 t/year (99.39%), and 6822 t/year (0.61%) was negative waste. Based on the results, the

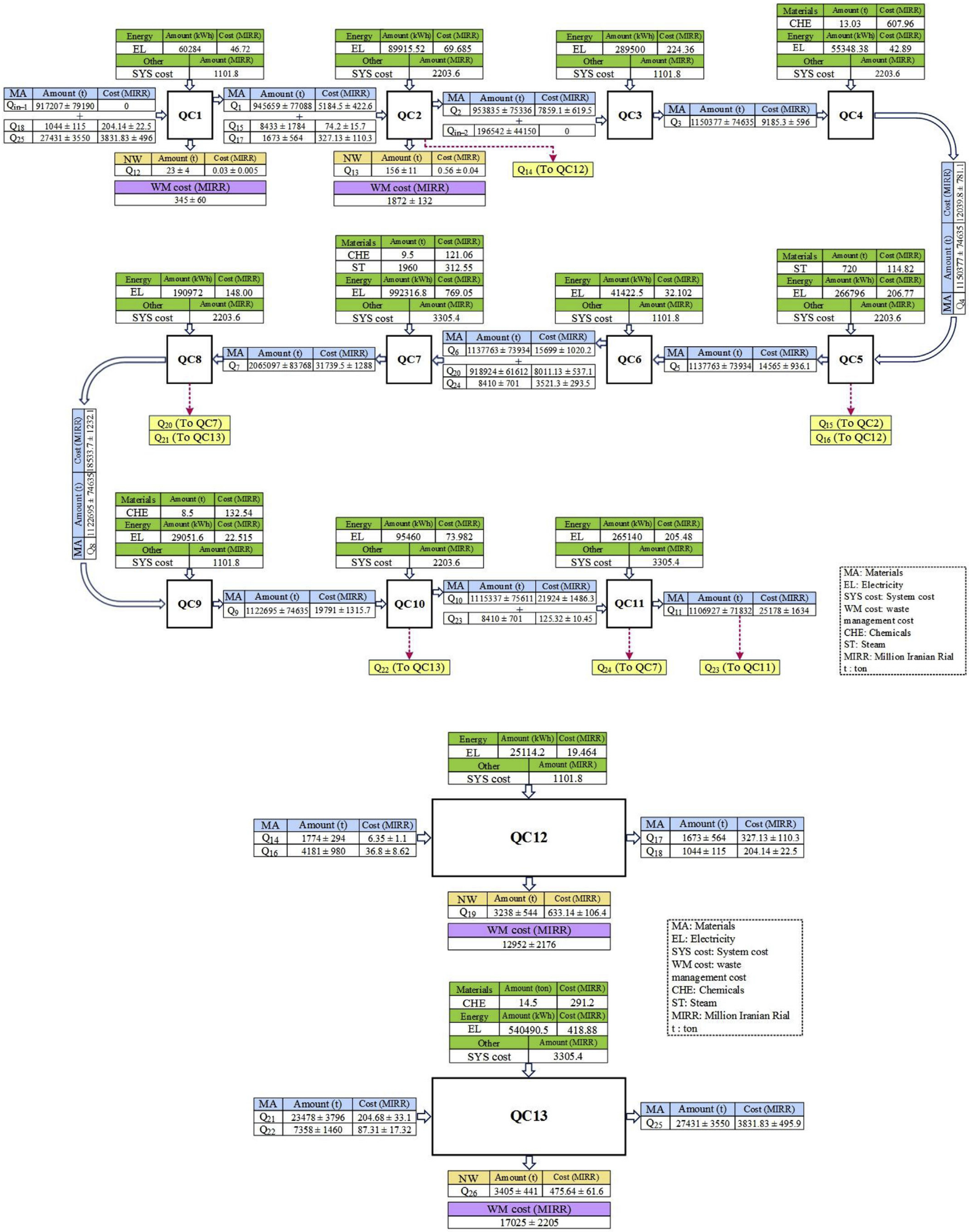

Fig. 4. Material flow cost accounting for petrochemical WWTP.

largest percentage of negative waste was waste sludge (49.91%) followed by slop oil (47.46%).

According to the MFCA results, 0.0561 Million Iranian Rials (MIRR) accounted for the total treatment cost per ton of inlet wastewater. The results showed that the total cost of the treatment system was 62497.23 MIRR; this figure consisted of energy cost (2279.9 MIRR; 3.65%), materials cost (1580.13 MIRR; 2.53%), system cost (26443.2 MIRR; 42.31%), and waste management cost (32194 MIRR; 51.51%). According to the results shown in Fig. 4, the positive product (treated wastewater) cost and negative waste cost were 25178 and 1109.37 MIRR, respectively. The system and waste management costs altogether comprised 93.82% of the total cost of the WWTP; therefore, the potential for improvement lies in these areas.

The allocations of energy, system, material, and waste management costs among the different QCs are presented in Fig. 5. From this figure, it can be clearly seen that among all the treatment steps, the waste sludge treatment unit accrues the highest percentage of treatment costs (33.67% of total treatment costs) followed by slop oil separation sump (22.52% of total treatment costs), the largest portion of which is associated with waste sludge management. It was recently proven that the expense for waste sludge treatment encompasses about 25%–60% of the total operational costs of WWTPs (Zhang et al., 2009). Thus, improving the waste management system can create a high potential for cost reduction.

The results of the current study showed that the highest percentage of energy costs (about 33.73% of the total energy costs) is found in the aeration unit (QC6) because of the existence of six sets of surface aerators with high energy consumption. The highest percentage of chemical cost (about 38.5% of the total material costs) is found in the coagulation and flocculation unit (QC4) followed by the aeration tank (about 27.4% of the total chemical cost). In the coagulation and flocculation unit, in addition to chemicals such as coagulants and polyelectrolytes, a considerable amount of neutralizers is used, and this increases the total chemical costs.

3.1.5. *Identification of improvement requirements*

The DR technique provides an accurate and reliable dataset for the decision-making process. Therefore, in this study, the reconciled data was used to provide improvement scenarios. MFCA results showed that the waste management system (especially biological waste management) imposes a high cost for WWTP. This gives a hint to the company managers looking for improvement opportunities to reduce the total cost of the system and movement towards sustainability. In the following, the selected improvement plans are introduced. These focus areas were proposed based on their effectiveness in reducing the total cost of the WWTP. Considering that the studied system is a full-scale WWTP, therefore, it is not feasible to apply major changes in the treatment system. However, by planning and implementation of management practices and upgrading the treatment processes, the total cost of the WWTP can be reduced. Accordingly, three improvement solutions were proposed, as follows: (1) Removal of the neutralization unit, (2) Minimization of excess activated sludge, and (3) Installation of a stripping system. The details of each proposed solution are provided below.

3.1.5.1. Removing the neutralization unit. A neutralization unit was designed to adjust the pH prior to the biological treatment system. It consisted of two compartments: one mixing tank coupled with a stirrer and one reaction tank. Even though the neutralization unit was considered as the pH adjusting step in the studied WWTP, this process is currently done in the primary coagulation unit (QC4), and the wastewater entering the biological system has optimum pH values. However, based on MFCA calculations, the neutralization unit accounts for approximately 1.81% of the total treatment and 1.41% of the total energy costs. This is because the stirrer is always working in the mixing tank. The solution to this proposes to shut down the neutralization unit which currently has no specific function in the treatment process. Based on the MFCA results, implementing this solution can result in a reduction of about 1133.9 MIRR (1.81%) in the total annual costs of the studied WWTP.

3.1.5.2. Minimization of excess activated sludge. The treatment and disposal process of the excess sludge generated from biological treatment processes represents a bottleneck in WWTPs and

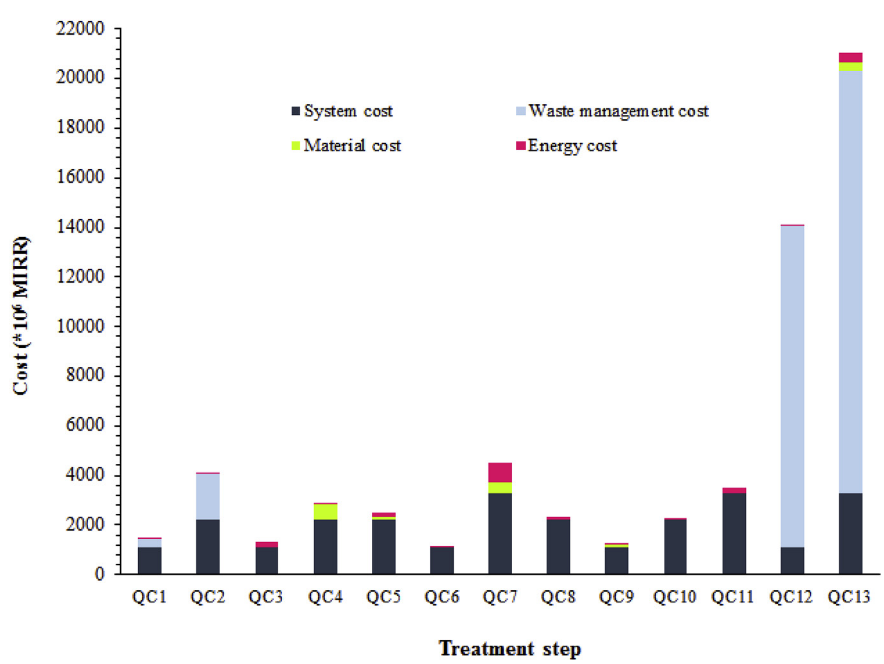

Fig. 5. The cost allocation for different treatment steps of petrochemical WWTP.

requires tremendous expenditures. Therefore, there is a great economic incentive for WWTPs to reduce waste sludge production (Rajesh Banu et al., 2019). Since the studied WWTP produces a high amount of waste activated sludge (about 30836 t/year) from primary and secondary clarifiers, the management cost of this waste stream (including treatment and disposal costs) is consequently very high, accounting for 33.67% (21040.5 MIRR) of the plant's total operating costs. Therefore, this is an important area which has a high potential for cost reduction.

In the present study, the method provided by Yasui et al. (1996) is proposed to reduce excess sludge production from a biological treatment system. This method was successfully applied in full-scale municipal and industrial WWTPs and showed no excess sludge to be withdrawn. With this technology, the waste activated sludge from the plant which should be disposed of is brought into contact with a sufficient concentration of ozone in order to oxidize and disintegrate the sludge. Then it is recirculated into a bio-treatment system to mineralize the particulate and soluble organic matters. The schematic flow-diagram of the proposed improvement plan is presented in Fig. S1 in the electronic supplementary material (ESM). It has been previously proven that the ozonation of waste activated sludge with an ozone concentration of 50 mg/g mixed liquor suspended solids (MLSS) can result in zero excess sludge production (Lee et al., 2005).

Based on local market surveys, the total investment and total operating cost per year for setting up a new ozonation unit with the production capacity of 500 g O_3/h were estimated to be about 10400 and 3412 MIRR, respectively. It is necessary to mention that an ozonation system with a capacity of 500 g O_3/h was selected based on the following factors: the volume of produced waste activated sludge in the plant (88 m^3/day), the MLSS content of waste activated sludge (2323 ± 1080 mg/L), and the ozone gas concentration of 50 mg O_3/g MLSS.

In addition to the installation cost of the ozonation system, the costs associated with the recirculation of ozonated sludge to the aeration tank should be considered. The influence of this improvement solution on the total mass balance and cost allocation in the selected WWTP is illustrated in Fig. S2 in the ESM. By launching this system, cost savings of 15548.22 MIRR (24.9%) annually can be achieved (considering five years amortization), because of the ability of the proposed solution to reduce energy consumption and excess sludge production. Considering the results, the implementation of this system can increase the percentage of positive products from 99.39% (1106927 t/year) to 99.7% (1110332 t/year) and decrease the negative wastes from 0.61% (6822 t/year) to 0.3% (3417 t/year). Moreover, by implementing this system, there will be no secondary air pollutants caused from the combustion of excess activated sludge in the incinerator.

3.1.5.3. Installation of stripping system. Wastewater generated from petrochemical complexes contains high concentrations of pollutants, mainly volatile organic compounds (VOCs) (Chirila et al., 2011). The emission of VOCs from wastewater treatment facilities is a concern because of their known and/or potential impact on the environment and human health (Yang et al., 2014). In accordance with Iranian National Environmental Standards (Shaeri and Rahmati, 2012), an industrial company that is detected as being a polluting industry must pay about 1% of its net annual sales as a surcharge for permit noncompliance with the emission standards. Hence, these compounds need to be controlled in the treatment plant to decrease their emissions and reduce the costs associated with the permit noncompliance surcharges.

For this case, a steam stripping system is proposed as an improvement solution. Steam stripping is a conventional method for physically separating VOCs from the liquid phase. The efficiency of the steam stripping system as a VOCs control option was reported to be about 92%–99% (Hassan and Timberlake, 1992; US-EPA, 1998). In our previous study (Behnami et al., 2018), we found the steam stripping system as an efficient and cost-effective VOCs controlling strategy in the petrochemical WWTP. Therefore, using a steam stripper as the VOCs separation technology in the inlet of WWTP can result in the VOCs emissions from downstream units meeting emission standards. However, the steam stripper's overhead vapor which contains water and organic compounds is introduced into the incinerator for final treatment. It is necessary to mention that the required steam is provided from the utility unit of the petrochemical plant, so there is no need for heating equipment.

Based on a local market survey, the total investment and operating costs for implementing a steam stripping system (5 years amortization) were estimated to be about 2800 and 15184 MIRR, respectively, both of which were considerably lower than the cost paid as a surcharge for permit noncompliance. It is noteworthy that in this case study, the surcharge costs were not included in the total cost of the WWTP; however, environmental penalties impose a

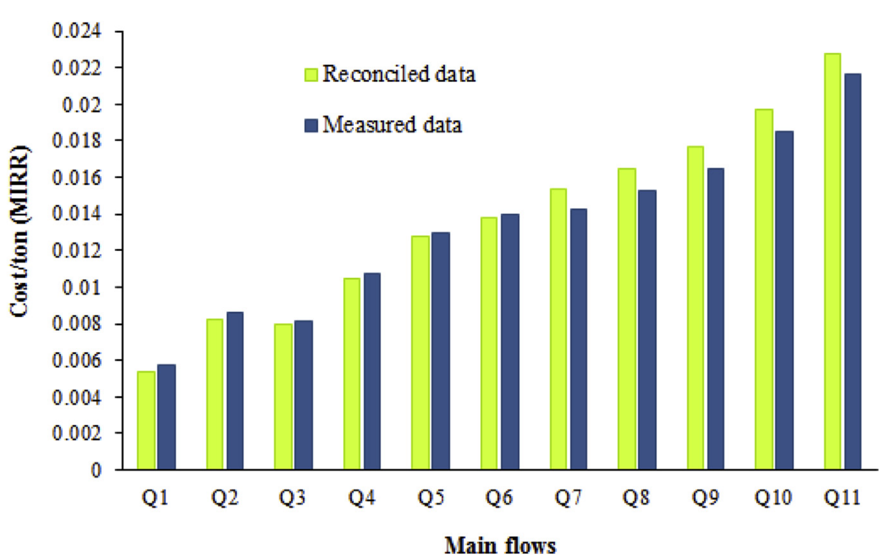

Fig. 6. The comparison of MFCA results for reconciled and unreconciled data.

high cost on companies, and such costs can be reduced by decreasing the pollutants emitted by implementing the improvement plans.

3.2. Preference of the proposed method

In this section, we try to show the importance of data reconciliation in MFCA calculations. For this purpose, we established MFCA calculations without considering step 4 in integrated approach presented in Fig. 2. The total imbalance observed in each QC varied from 0% to 10.35%, which makes mass balance never to be closed. The material flow cost accounting of the WWTP based on measured data (unreconciled data) is shown in Fig. S3 in the ESM.

The comparison of the total cost per ton of various flow streams for reconciled data and measured data (unreconciled) is illustrated in Fig. 6.

The result indicates a relatively significant difference between MFCA results for reconciled and measured data (unreconciled). For example, there is about 5.1% difference between total cost of final effluent (Q11) for reconciled and unreconciled data, and for other flow streams, the difference was calculated 1.5%–7.4%. Obviously, MFCA calculations using these unreconciled data lead to enormous errors, which can affect the management practices and decision-making process. Hence, this study introduces the integrated approach of data reconciliation, and material flow cost accounting in order to enhance the accuracy and certainty of data prior to mass balance calculations and MFCA implementation.

4. Conclusions

4.1. General conclusions

Poor quality of process data leads to large errors in establishing an accurate mass balance and consequently material flow cost accounting in a system such as WWTP. Hence, the present work has introduced a novel practical stepwise approach to enhancing the reliability and consistency of data intended for use in MFCA calculations and decision-making processes. This approach uses the data reconciliation technique to improve the accuracy and certainty of measurements. A full-scale petrochemical wastewater treatment plant was selected for the establishment of this integrated approach. The most obvious findings can be summarized as:

- An error of −3.22% (−35244 t/year) between total input and output streams of WWTP was observed, demonstrating mass imbalance in the system.
- After simultaneously solving the incidence matrix (system of balances), the error of reconciled data was equal to zero, causing the mass balance to be closed.
- By including the data reconciliation into MFCA, an accurate mass balance can be established in the system; this is a crucial requirement for accurately implementing MFCA in a system.
- The comparison results showed a relatively significant difference between material flow cost accounting for reconciled and unreconciled data (measured data).
- The application of this novel integrated approach enables decision-makers to more confidently enhance both financial and environmental performance and define appropriate improvement solutions for a system.

4.2. Implications for theory and practice of cleaner production/sustainability

Concerning the implications for theory and practice, this study opens a new perspective in material flow cost accounting. Until now, no research has been done to investigate the integrated approach of data reconciliation and material flow cost accounting. This novel approach provides an evidence that including data reconciliation into material flow cost accounting can result in accurate and reliable material flow cost accounting outcomes. In turn, the findings of this study have important implications for decision-making processes. Because using this approach help decision-makers to get closer from the imbalanced to the real data, thereby increasing the transparency of the real costs of various streams and providing improvement plans more confidently. Therefore, this study contributes to literature on cleaner production and sustainability.

Conflicts of interest

The authors confirm that there is no competing interest in this research.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2019.01.218.

Nomenclature

Abbreviations

MFCA	Material flow cost accounting
WWTP	Wastewater treatment plant
EMA	Environmental management accounting
ERP	Enterprise resource planning
EMS	Environmental management systems
DOE	Design of experiments
DR	Data reconciliation
TPC	Tabriz petrochemical company
API	American petroleum institute
DAF	Dissolved air flotation
QC	Quantity center
RSD	Relative standard deviations
MIRR	Million Iranian Rials
ESM	Electronic supplementary material
MLSS	Mixed liquor suspended solids
VOCs	Volatile organic compounds

Sets

MA	Materials
EL	Electricity
SYS	System cost
WM	Waste management
CHE	Chemicals
ST	Steam
t	Index for tone
n	Index for input materials
p	Index for desired products
w	Index for wasted materials

e Index for energy
s Index for system

Parameters

I_i Mass of input material
P_j Mass of desired product
W_k Mass of wasted material
E_e Amount of energy types e required in a process
S_s Required amount of sth item involved in a process
C_{pc} Total cost of process
C_{mat} Material costs
C_{engy} Energy costs
C_{sys} System costs
C_{wm} Waste management cost
C_{mat_i} Unit cost of input material i
C_{engy_e} Unit cost of energy types e
C_{sys_s} Unit cost of sth item
C_{wm_k} Unit cost for management of kth waste materials
y Vector of measurements
x Vector of true value of measured variables
ε Measurement random errors
σ Standard deviation
ψ Covariance matrix of measurement errors
A Matrix of linear constraints
λ Lagrange multipliers
L Lagrange function

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