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Automated targeting for conventional and bilateral property-based resource conservation network

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ABSTRACT

Resource conservation is an effective way to reduce operation cost and to maintain business sustainability. Most previous works have been restricted to "chemo-centric" or concentration-based systems where the characterisation of the streams and constraints on the process sinks are described in terms of the concentration of pollutants. However, there are many applications in which stream quality is characterised by physical or chemical properties rather than pollutant concentration. In this work, the automated targeting approach originally developed for the synthesis of composition-based resource conservation network is extended for property-based network. In particular, targeting for the property-based networks with process modification and interception processes are addressed. Based on the concept of insight-based targeting approach, the automated targeting technique is formulated as a linear programming (LP) model for which the global optimum is guaranteed if a solution exists. In case(s) where process modification is involved, the automated targeting technique is formulated as a non-linear programming (NLP) model, in which is solved globally by commercial optimisation software. In addition, a new approach for the bilateral property integration problem is also presented in this work. Literature and industrial case studies are solved to illustrate the proposed approach.

1. Introduction

In the past decades, process industries have been focusing on conventional end-of-pipe waste treatment in order to comply with environmental legislation. However, recent trend shows that the industries are now diverging towards the reduction of the generated waste and the search for better alternatives in securing sustainable manufacturing processes. This is mainly due to the increase of public awareness towards environmental sustainability, the raise of manufacturing cost (i.e. raw material, utilities, end-of-pipe waste treatment, etc.) as well as the more stringent environmental legislation. One of the cost effective solutions in responding to the above needs is resource conservation activities where materials are reused/recycled within processes without adversely affecting the process performance. In this regard, process integration has been commonly accepted as an effective tool in evaluating various resource conservation alternatives.

El-Halwagi [1,2] defined process integration as *a holistic approach to process design, retrofitting and operation which emphasises the unity of the process*. In most cases, both fresh material consumption and waste generation are reduced simultaneously by carrying out resource conservation activities [1–4]. Over the past decade, extensive works have been reported for the synthesis of water and utility gas (mainly on hydrogen integration) networks as special cases of *mass integration*, ranging from both insight-based [5–30] and mathematical optimisation approaches [31–52].

The seminal work of insight-based approach for water network synthesis was proposed by Wang and Smith [5], focusing on mass-transfer processes (often known as the *fixed load problem*). The authors presented the limiting composite curve to locate the minimum water flowrates, i.e. fresh water consumption and wastewater generation, prior to detailed network design. Later, the proposed work was extended to cases where regeneration processes are used to purify process streams before they are further reused/recycled [6–8]. Later works in this area investigated the more generalised *fixed flowrate problem* where non-mass transfer processes are considered [9–24]. In addition, the early works in mathematical optimisation approaches for water network synthesis were reported by Takama et al. [31,32]. Later works on this

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technique may be broadly categorised as deterministic [33–44] and stochastic optimisation [45–49] approaches.

On the other hand, various insight-based targeting techniques were developed for utility gas network synthesis such as value composite curves [25], hydrogen surplus diagram [26,30], material recovery pinch diagram [12,29], limiting composite curves [16] and cascade analysis technique [27]. Besides, the use of mathematical optimisation approaches has also been reported for utility gas network synthesis [50–52].

It is worth mentioning that the combined use of both insight-based and mathematical optimisation techniques were also reported [53–56]. Among these, the automated targeting approach by Ng et al. [56] incorporates the targeting concept of insight-based technique into the mathematical optimisation model to locate the minimum flowrate/cost targets for a resource conservation network (RCN). The flexibility in changing the objective function is one of the advantages of the automated targeting approach over the conventional insight-based techniques. In addition, automated targeting still provides similar insights for process design that can be drawn from the insight-based techniques.

Notwithstanding the importance of mass integration, the previous proposed approaches are limited to address problems that characterise process streams in terms of pollutant concentration. However, design specifications are based on the satisfaction of stream property constraints in many cases [57–59]. For instance, the design and performance of a paper-making machine is based on the properties of reflectivity, opacity, or density; rather than the composition of paper [59]. In addition, effluent legislation is often defined in term of properties (e.g. pH, turbidity, toxicity, colour) apart from pollutant concentration (e.g. COD, suspended solids, etc.). In order to address design problems that are governed by functionalities and properties, the framework of *property integration* was introduced by El-Halwagi and co-workers [57–63]. El-Halwagi et al. [57] defined property integration as *a functionality-based, holistic approach to the allocation and manipulation of streams and processing units, which is based on the tracking, adjustment, assignment, and matching of functionalities throughout the process*.

Shelley and El-Halwagi [58] developed the concept of property-based clusters to enable the tracking of properties in a RCN. Later, El-Halwagi et al. [57] presented a visualised tool to design property-based RCN with three properties. Next, Kazantzi and El-Halwagi [59] presented graphical approaches to locate minimum resource consumption targets for a reuse/recycle scheme. Besides, process modification has been considered by Kazantzi and El-Halwagi [59]. Algebraic tools were later developed to locate rigorous targets for single [60] and multiple properties [61]. Recent works also reported the extension of the developed techniques to dynamic systems [62,63].

In this work, the automated targeting technique that was proposed for the synthesis of mass exchange network [1] and concentration-based RCN [56] is extended for locating the minimum flowrate/cost targets for a property-based RCN. Besides, process modification and pre-treatment system are explored; where the latter scenario has not been previously reported [57–63]. Another new variant of the *bilateral property integration problem* is also introduced in which the property operator values of the process sinks and sources exist in between the property operator values of external fresh resources. This concept is important whenever a nominal desired or targeted sink property operator value exists that is neither being the highest (superior) nor the lowest (inferior) to other operator values of the process sources and sinks, as in the conventional cases [59,60]. In other words, the situation is different from the conventional cases where one is simply trying to minimise the *single* fresh resource that has a property value that is either superior or inferior to other process sources and sinks. For instance, a sink may be characterised by pH with a nominal desired value of 7 (neutral); while the pH values of the process sources may be higher and lower than this desired value. Hence, sources with pH close to 7 are considered as high quality, while sources with pH far above or below 7 are regarded as poor quality.

2. Problem statement

The problem for a RCN with single property may be stated as follows:

Given a set of N_{sources} sources in a process. Each process source is process stream that may be considered for reuse/recycle or discharge. Each source has a flowrate, F_i and is characterised by a property p_i. Given also a set of N_{sinks} process sinks that are process units that can accept sources. Each sink requires a flowrate, F_j and an admissible inlet property, p_j from the source(s), which complies with the predetermined allowable property constraints as follows:

$$p_j^{\min} \le p_j \le p_j^{\max} \tag{1}$$

where $p_j^{\min}$ and $p_j^{\max}$ are the specified lower and upper bounds of the admissible properties to sink j. Besides, a set of N_{fresh} external fresh resources may be purchased to fulfil the requirement of the sink(s). In most cases, the property values of the fresh resources are either being superior or inferior to other property operators of the sinks and sources [59,60]. Hence, this can be considered as a *single-sided* property integration problem, as only fresh resource of either end of the property operator level is being minimised. In this work, a *dual-sided* case is introduced, where two high-quality fresh resources are to be minimised, and one of these exists at the highest property operator value, while the other exists at the lowest property operator level. This variant of problem is termed as *bilateral property integration*.

A general linearised property mixing rule is needed to define all possible mixing patterns among the individual properties. One such form of mixing rule takes the following expression [58]:

$$\psi(\bar{p}) = \sum_i x_i\, \psi(p_i) \tag{2}$$

where $\psi(p_i)$ and $\psi(\bar{p})$ are operators on source property p_i and mixture property $\bar{p}$, respectively; while x_i is the fractional contribution of stream i in the total mixture flowrate.

The objective of this work is to locate the minimum flowrate/cost targets for a property-based RCN prior to detailed design. Different scenarios are analysed. This includes direct material reuse/recycle, process modification, as well as the placement of interception and pre-treatment systems. Literature and industrial case studies are solved to illustrate the proposed approach.

3. Automated targeting approach

The automated targeting technique was originally developed by El-Halwagi [1] for mass exchanger network synthesis. Recently, Ng et al. [56] extended the approach for synthesis of composition-based RCN based on the concept of algebraic targeting technique of cascade analysis [13,17], with the removal of the dual-step procedure. It is worth noting that in all cascade analysis techniques, infeasible cascades with material flow balances are first generated to determine the largest material deficit, which is then added as fresh resource in the second step to remove all deficits and yield a feasible material cascade. Successful application is seen in water network [13,15,17,20,21,24], utility gas network [27] and

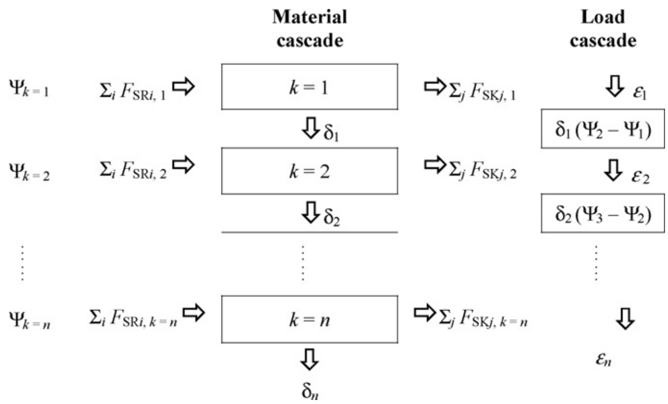

Fig. 1. Property interval diagram.

property-based network synthesis [60]. Via the proposed automated targeting approach, the two-step targeting approach is readily removed. In this work, the automated targeting is adapted for a property-based RCN.

The procedure for the automated targeting technique for a property-based RCN is next illustrated. A revised *property interval diagram* [2,60] is first constructed, where the property operators (Ψ_k) of the material sinks and sources are arranged in an ascending order, from the lowest level $k=1$ to the highest level $k=n$, as shown in Fig. 1. In cases where the property operator levels for fresh resource(s) and zero property operator level that do not exist within the process sinks and sources, an additional property operator level of zero is added. Besides, an arbitrary value is added at the final level (highest among all property operators) of the property interval diagram to allow the calculation of residual property load.

Next, *material flowrate cascading* is performed across all property operator levels. At each property operator level k, the flowrate difference between the total available material sinks and sources ($\Sigma_i F_{SRi} - \Sigma_j F_{SKj}$) is determined. Eq. (3) shows the *net material flowrate* of each k-th level (δ_k). As shown, δ_k is the summation of the net material flowrate cascaded from the earlier property operator level ($k-1$), δ_{k-1} with the flowrate balance at property operator level k, $(\Sigma_i F_{SRi} - \Sigma_j F_{SKj})_k$, i.e.:

$$\delta_k = \delta_{k-1} + \left(\sum_i F_{SRi} - \sum_j F_{SKj} \right)_k \tag{3}$$

Note that the net material flowrate (δ_k) can either take positive or negative value, with positive value indicates material that flows from the lower into higher level and vice versa. This is in agreement with the cascade analysis technique [13,17,60].

Apart from material flowrate cascading, *property load cascade* is also essential to ensure a feasible RCN. The calculation for property load cascade from level $k-1$ to level k is performed as follows. Within each property operator interval, the property load is given by the product of the net material flowrate from level k (δ_k) and the difference between two adjacent property operator levels ($\Psi_{k+1} - \Psi_k$). Similar to the material flowrate cascade [13,17], *residual property load* of each concentration level k (ε_k) is to be cascaded down to the next property operator level [60]. Hence, property load balance at the k-th operator level is determined by the following equation:

$$\varepsilon_k = \varepsilon_{k-1} + \delta_k(\Psi_{k+1} - \Psi_k) \tag{4}$$

where ε_{k-1} is the residual property load cascaded from operator level $k-1$.

In order to ensure that the maximum allowable property load (i.e. minimum acceptable stream quality) of sinks in each level is fulfilled, the property load that is transferred from lower to higher level, i.e. the residual property load, ε_k must take a positive value. Therefore, Eq. (5) is included as a constraint in the optimisation model. Note also that, a pinch point (represents the overall bottleneck for the RCN problem) is observed where zero residual property load is located in the property load cascade:

$$\varepsilon_k \geq 0 \tag{5}$$

The automated targeting approach will now be applied to various property-based RCN problems.

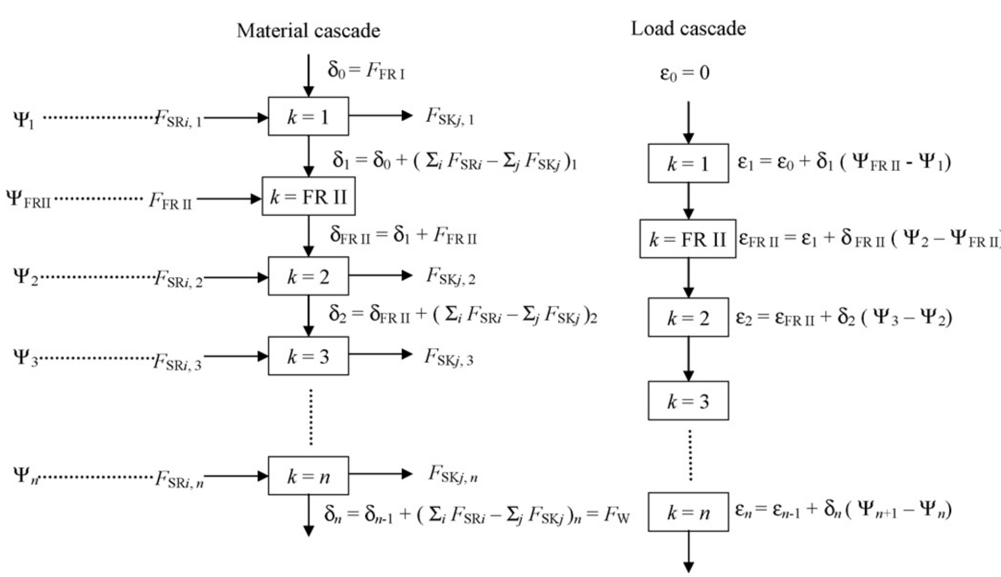

Fig. 2. Generic PCD for direct reuse/recycle.

4. Direct reuse/recycle

In order to target the minimum fresh resource and waste flowrates for a direct reuse/recycle scheme, the property interval diagram may be converted to a *property cascade diagram* (PCD) as in Fig. 2. Following the proposed procedure, the property operators of all process sinks and sources are first arranged in an ascending order as shown in Fig. 2. Next, the net material flowrate of each property operator level k (δ_k) is determined using Eq. (3). Note that the net material flowrate found before the first property operator (δ_0) and final property operator (δ_k) levels corresponds to the fresh resource (F_{FR}) and waste discharge (F_W) flowrates for the network, respectively (Fig. 2). These values are the results of the automated targeting technique. In most cases, the fresh resource possesses the highest quality, and corresponds to zero property operator. In cases where the fresh resource does not exist at the zero operator value, a new property operator level ($\Psi_{FR\,II}$) is to be added (see Fig. 2).

For a property-based RCN with single fresh resource, the optimisation objective is formulated as to minimise the fresh resource flowrate (F_{FR}), given as in the following equation:

$$\text{Minimise } F_{FR} \tag{6}$$

In cases where the RCN is served by multiple fresh resources, the optimisation objectives can be set to determine the overall minimum fresh resources (Eq. (7)) or their minimum total operating cost (TOC, Eq. (8)).

$$\text{Minimise } \sum_z F_{FR,z} \tag{7}$$

where $F_{FR,z}$ is the flowrate for fresh source z.

$$\text{Minimise } \text{TOC} = \sum_z C_{FR,z} \times F_{FR,z} \tag{8}$$

where $C_{FR,z}$ is the operating cost of z-th fresh resources. The flexibility in changing the objective function is one of the advantages of the automated targeting approach over conventional insight-based techniques, e.g. [59,60]. One may also set to minimise the total annualised cost of the RCN, if the design scenario calls for the inclusion of the capital costs. Example 1 is now used to illustrate the proposed technique.

5. Example 1

Fig. 3 shows a metal degreasing process [59] that is used to illustrate the automated targeting approach. As shown, fresh organic solvent is used in the degreaser that employs reactive thermal processing to decompose grease and organic additives. The liquid solvent is then regenerated and recycled to the degreaser; while the offgas containing solvent is passed through a condenser and an absorber (where fresh solvent is also used) before being flared. Besides, another offgas stream leaving the degreaser is also passed through a condenser before it is sent to the flare unit. The two condensate streams from the solvent regeneration unit (SR1) and the degreaser (SR2) are regarded as process sources where reuse/recycle may be considered in order to reduce the consumption of the fresh solvent. In this case, two process sinks (where solvent is consumed) are easily identified, i.e. degreaser (SK1) and absorber (SK2).

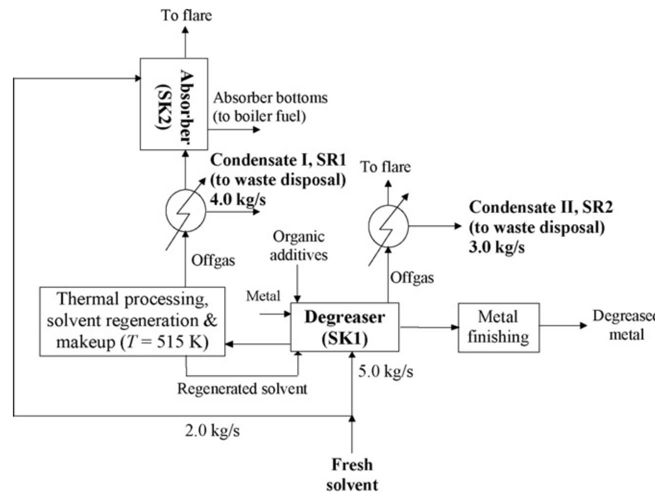

Fig. 3. Schematic flowsheet of metal degreasing process [59].

The main property of the solvent that dictates the extent of reuse/recycle of the process sources is identified as Reid vapour pressure (RVP), which is important in characterising the volatility (and, indirectly, the composition) of the solvent. The general mixing rule for the RVP is given as follows [59]:

$$\overline{\text{RVP}}^{1.44} = \sum_i x_i \,\text{RVP}_i^{1.44} \tag{9}$$

The property operator for RVP, Ψ(RVP), can thus be expressed as follows:

$$\Psi(\text{RVP}_i) = \text{RVP}_i^{1.44} \tag{10}$$

Table 1 shows the limiting data for Example 1. In order to determine the minimum flowrate of the fresh solvent, Eq. (6) is optimised subject to the constraints given in Eqs. (3)–(5). Solving the LP model resulted in the PCD as shown in Fig. 4. Note that, a zero property operator ($\Psi_1 = 0\,\text{atm}^{1.44}$) is added in the first level of PCD as none of the sink or source comes with zero property operator. On the other hand, an arbitrarily high property operator value (in this case $\Psi_7 = 100\,\text{atm}^{1.44}$) is added at the last level of PCD to allow the residual property load (ε_6) to be computed. As shown in Fig. 4, the fresh (F_{FR}) and waste solvent (F_W) flowrates are both targeted as 2.38 kg/s, matching the previous reported results [28,59,60]. In this case, the pinch point is identified as 13.2 atm$^{1.44}$, where zero residual property load ($\varepsilon_5 = 0$) is observed. The network design for this case is shown in Fig. 5, designed using Nearest Neighbour Algorithm [14] that was originally developed for concentration-based RCN.

Table 1
Limiting data for Example 1 [59,60].

Process	Flowrate (kg/s)	Reid vapour pressure, RVP (atm)	Property operator, Ψ (atm$^{1.44}$)
Sink			
Degreaser (SK1)	5.0	3.0	4.87
Absorber (SK2)	2.0	4.0	7.36
Source			
Condensate I (SR1)	4.0	6.0	13.2
Condensate II (SR2)	3.0	2.5	3.74
Fresh solvent	To be determined	2.0	2.71

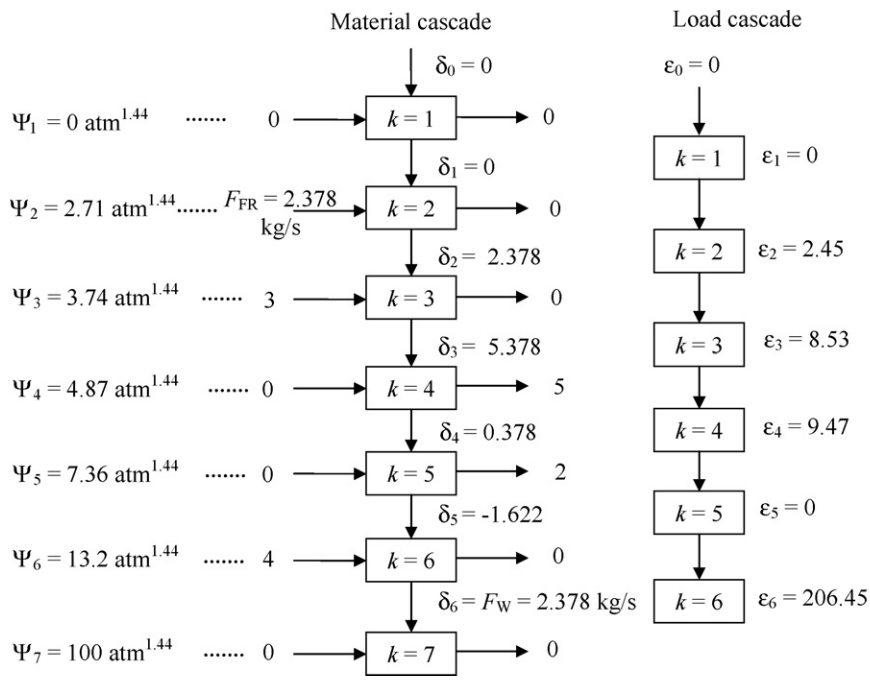

Fig. 4. PCD for Example 1.

6. Process modification and interception

After material recovery potential via reuse/recycle is exhausted, *process modification* and *interception* are effective means for further recovery of process source(s) for the reduction of fresh resource consumption [1,2,59,60,62,63]. Specifically, the operating conditions of individual processes are changed to give more desirable stream properties and/or flowrates for further recovery. Example 1 is used to demonstrate the extension of the automated targeting approach for process modification. Next, material recovery in a palm oil milling processes with interception placement (Example 2) is solved to illustrate the proposed approach.

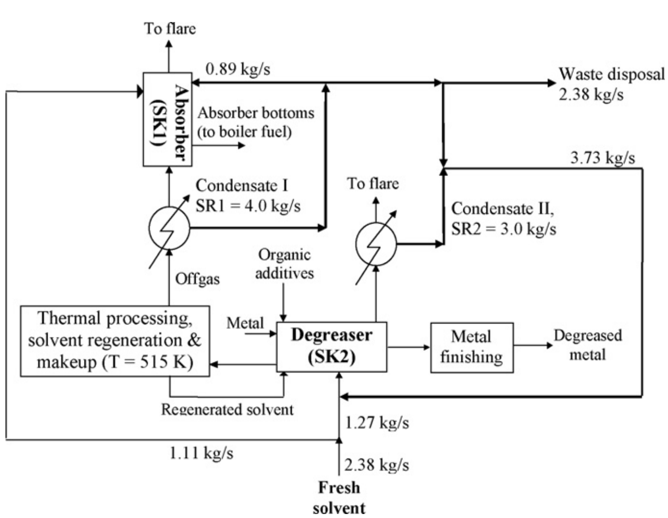

Fig. 5. Network design for metal degreasing process with solvent reuse/recycle (Example 1).

7. Example 1 (revisited)

According to Kazantzi and El-Halwagi [59], the RVP for the condensate from solvent regeneration unit (SR1) is a function of thermal regeneration temperature:

$$RVP_{SR1} = 0.56 \times e^{((T-100)/175)} \quad (11)$$

where T is the temperature of the thermal processing system in Kelvin (K). The acceptable operating temperature for this operation ranges between 430 K and 520 K [59]. At present, the thermal processing system operates at 515 K, resulting in an RVP of 6.0 atm. This operating condition can be modified to enable more solvent from SR1 to be reused/recycled to the two process sinks (SK1 and SK2).

Based on Eq. (11), the lowest and highest RVP values for SR1 are calculated as 3.69 atm (T = 430 K) and 6.17 atm (T = 520 K) respectively. The range of property operator is then determined as 6.56 $atm^{1.44}$ and 13.75 $atm^{1.44}$ using Eq. (10). In order to perform automated targeting, the property operators are first arranged in an ascending order. It is then observed that the property operator of SK2 (7.36 $atm^{1.44}$) falls within the property operator range of SR1. Since the arrangement of property operator levels are required before optimisation may be carried out, two new property operator levels (Ψ_5 and Ψ_7 for RVP_I and RVP_{II}, respectively) are added as variables in the PCD (Fig. 6) with its lower and upper limits given as in Eqs. (12) and (13). This allows material flowrate and property load cascades to be performed across the property operator level where SK2 exists. The new constraints given by Eqs. (12) and (13) allow the optimisation model to search for the optimum thermal regeneration temperature and RVP of SR1 within the range of 6.56–13.75 $atm^{1.44}$:

$$6.56\,atm^{1.44} \le RVP_I < 7.36\,atm^{1.44} \quad (12)$$

$$7.36\,atm^{1.44} < RVP_{II} \le 13.75\,atm^{1.44} \quad (13)$$

In addition, Eqs. (10) and (11) are added as process constraints in the optimisation model. Since the solvent regeneration unit can

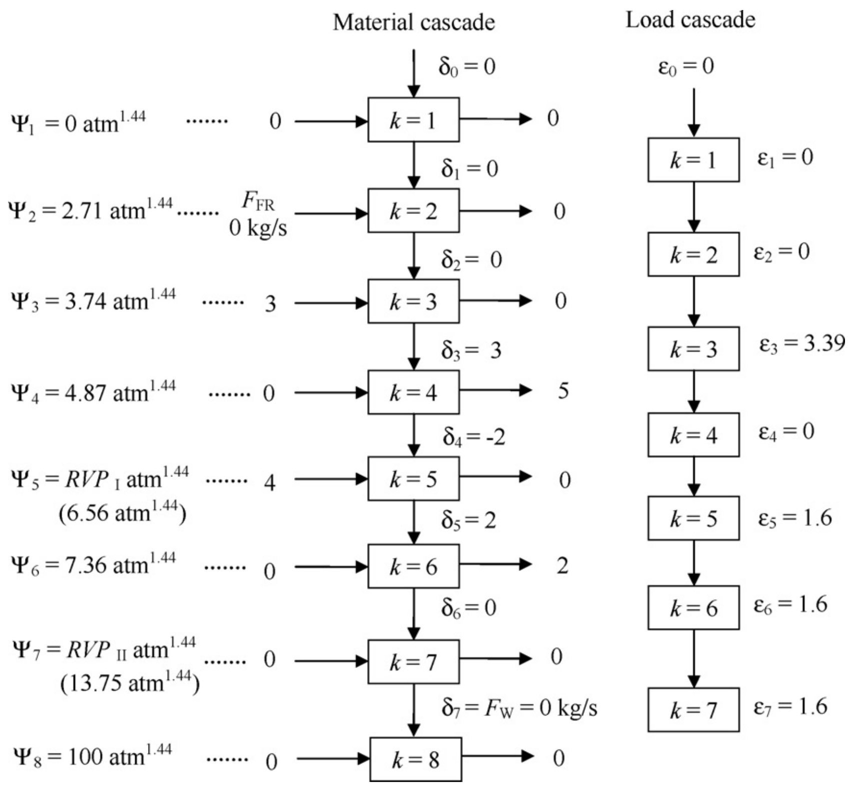

Fig. 6. PCD for Example 1 (with process modification).

only operate at one optimal temperature level; it is essential to restrict the flowrate of SR1 to appear either in Ψ_5 or Ψ_7, but not both simultaneously. Hence, the following constraints are added:

$$F_{SR1,\Psi 5} \times F_{SR1,\Psi 7} = 0 \quad (14)$$

$$F_{SR1,\Psi 5} + F_{SR1,\Psi 7} = 4 \quad (15)$$

where $F_{SR1,\Psi 5}$ and $F_{SR1,\Psi 7}$ are SR1 flowrates that are located in Ψ_5 and Ψ_7, respectively. While Eq. (14) sets either of these flowrate to zero; Eq. (15) indicates that the summation of these flowrates leads to the total available flowrate of SR1, i.e. 4 kg/s.

Although the above optimisation model is a NLP problem (due to the bilinear term in Eq. (14)); it can be optimised to achieve global optimality by commercial optimisation software (extended LINGO version 10.0 with a global solver is used in this work). The PCD for Example 1 with process modification is shown in Fig. 6. It is interesting to note that no fresh solvent is needed, and no waste solvent is discharged from the network when the thermal regeneration temperature is set as 430 K (corresponds to the optimal property operator of 6.56 $atm^{1.44}$). This is in agreement with the previous reported result in which graphical [59] and algebraic [60] approaches are used to solve the problem, respectively. However, in these earlier works, the exploration of process modification requires back calculation of the maximum acceptable property operator for both the degreaser and absorber, before the fresh resource and waste targets are determined. This limitation is readily overcome by the automated targeting approach where the optimal thermal regeneration temperature, minimum fresh resource and waste targets are located simultaneously. The optimal network that achieves the zero discharge and zero fresh targets is shown in Fig. 7.

8. Example 2

Fig. 8 shows a schematic flowsheet for a typical palm oil milling process [64]. In the crude palm oil (CPO) production section, the fresh fruit brunches (FFBs) are first sterilised in a high pressure vessel, before the sterilised fruits are separated from the bunches via a mechanical stripping process. The empty fruit brunches (EFBs) are normally used as fuel or further processed into fertiliser. The fresh fruit is digested and pressed in order to extract the crude oil. The extracted mixture is then sent to oil separation section for water removal (added during sterilisation and pressing). Apart from CPO, a low grade oil is also produced in the oil separation sec-

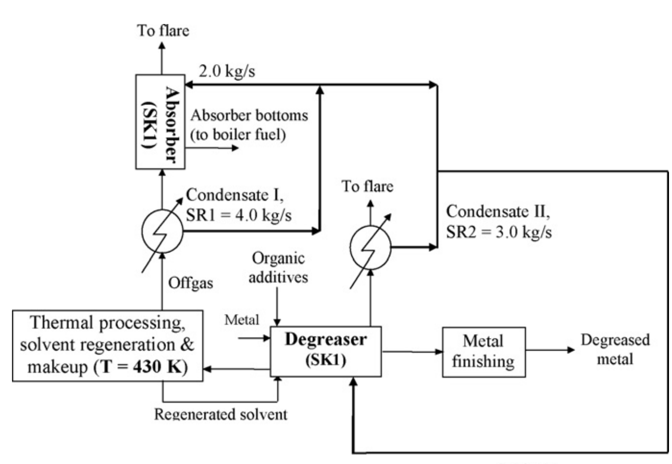

Fig. 7. Optimal network design for metal degreasing process after process modification [59,60].

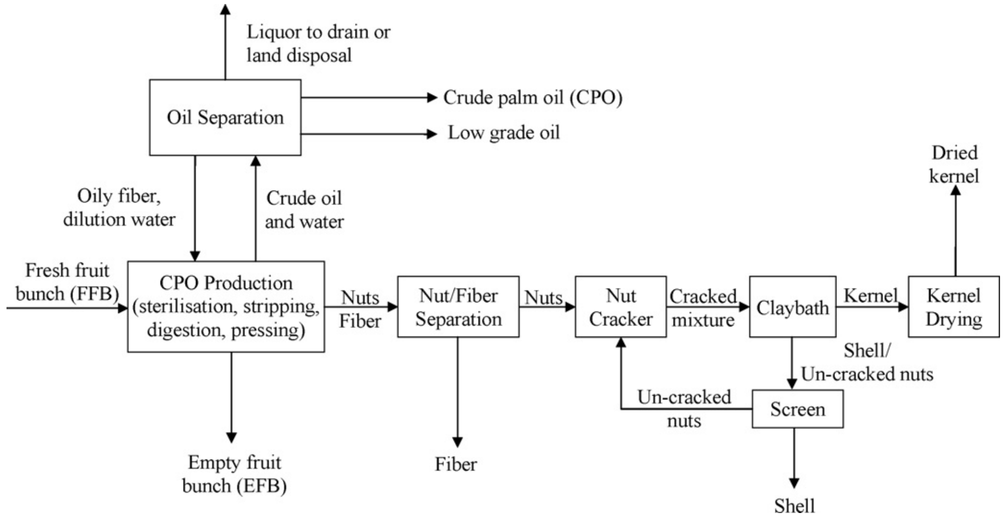

Fig. 8. Schematic flowsheet for a palm oil milling process [64].

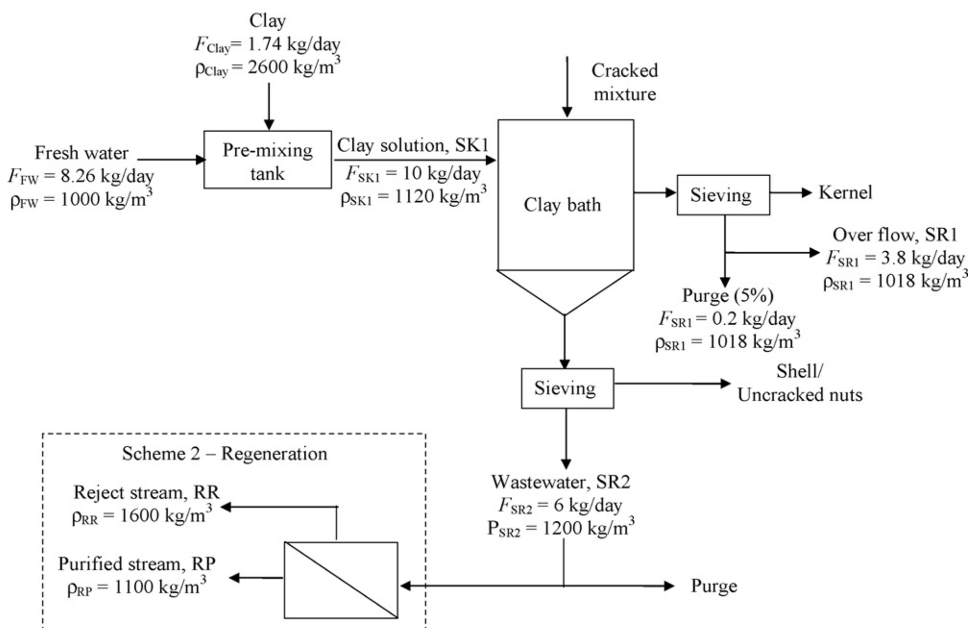

Fig. 9. Schematic diagram of clay bath.

Table 2
Limiting data for Example 2.

Process	Flowrate (kg/day)	Density, ρ (kg/m^3)	Property operator, Ψ (ρ) ($\times 10^{-4}$ m^3/kg)
Sink			
Clay solution (SK1)	10	1120	8.93
Source			
Scheme 1—recycling			
Over flow (SR1)	3.8	1018	9.82
Scheme 2—treatment			
Over flow (SR1)	3.8	1018	9.82
Bottom flow (SR2)	5.7	1200	8.33
Rejected stream (RR)	To be determined	1600	6.25
Purified stream (RP)	To be determined	1100	9.09
Fresh water (FW)	To be determined	1000	10
Clay	To be determined	2600	3.85

tion. The waste liquor is then sent for final treatment and eventual disposal.

Nuts and fibre are side products from CPO production. They are sent for further processing as another high quality oil can be extracted within the nuts. Fibres are first separated from the nuts, before the nuts are sent for cracking. Upon cracking, the cracked mixture, mainly consists of shell and kernel as well as some un-cracked nuts are separated in a clay bath based on flotation principle. Due to the different densities of the kernel (1070 kg/m^3), shell and un-cracked nuts (both approximately range between 1150 kg/m^3 and 1200 kg/m^3), a clay bath that operates with suspension density range of 1120 kg/m^3 allows the kernel to float and separated as the top stream [64]. The shell fractions as well as the un-cracked nuts with higher density are withdrawn from the bottom stream. The kernels are then dried and sold off as a by-product from the palm oil mill. Meanwhile, the shell and un-cracked nuts are separated in the screening process. The un-cracked nuts are sent back to nut cracker, while the shell is used as fuel.

In this work, water recovery for clay bath system is explored. A more detailed schematic diagram of the clay bath operation is shown in Fig. 9. The clay bath consists of slurry water whose proportions are chosen to achieve the desired density. However, the quality of the slurry degrades during use through inadvertent separation of the clay particles from water. Besides, the cracked mixture consists of impurities that affect the density of the solution in the clay bath. Therefore, make-up water and fresh clay are fed into the system to compensate for losses and to maintain the separation efficiency. As shown in Fig. 9, fresh water and clay are fed to the pre-mixing tank to prepare the clay solution with a desired density of 1120 kg/m^3 before it is fed to the clay bath. The cracked mixture is separated in the clay bath, where the "lighter" kernel flows out from clay bath with an over flow stream; while the "heavier" shell and un-cracked nuts are discharged from the bottom stream. Sieving is used in both over flow and bottom streams to separate the solids (kernel, shell and un-cracked nuts) from the liquid portion. Due to environmental concern, recovery of the two wastewater streams will be considered.

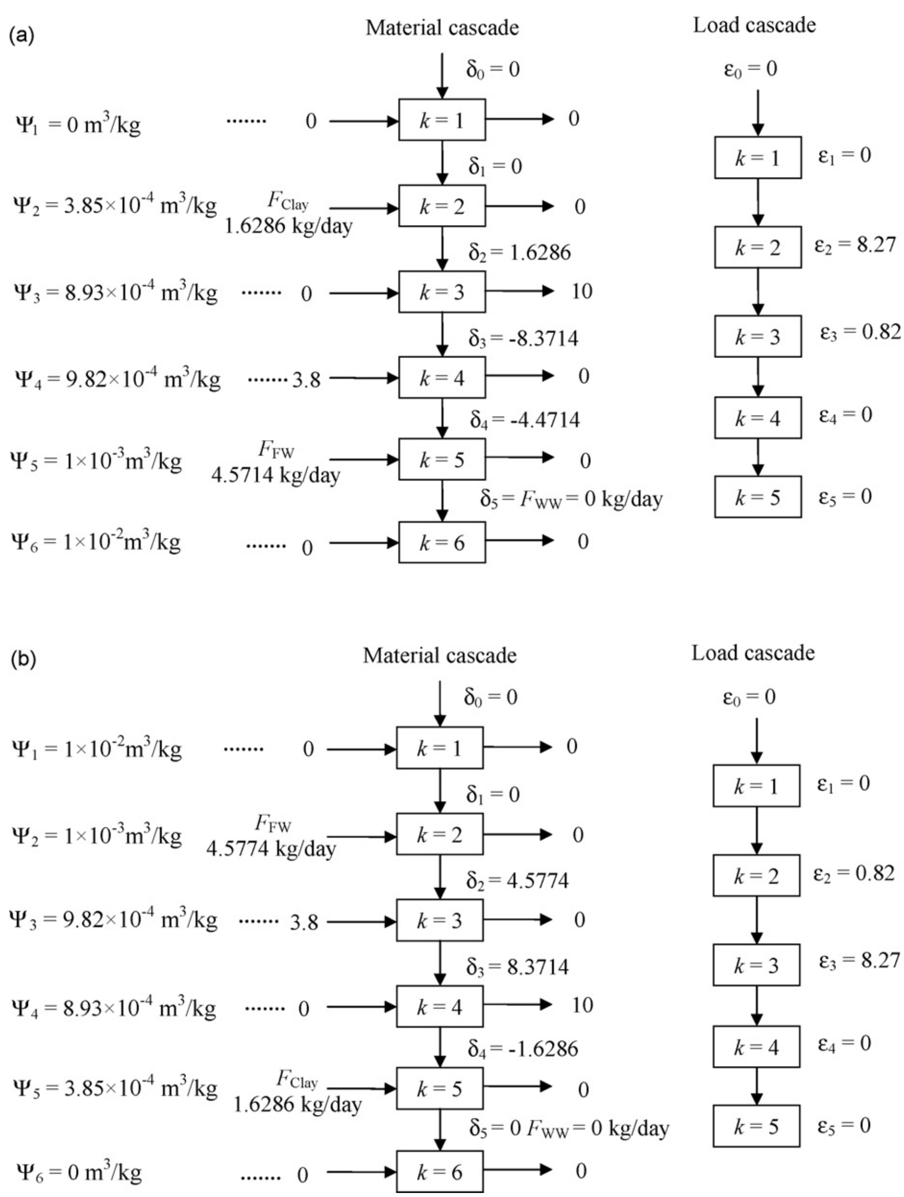

Fig. 10. (a) Superior cascade for Example 2 (Scheme 1). (b) Inferior cascade for Example 2 (Scheme 1).

Two water recovery schemes are analysed in this work. In the first scheme, water recycling from the clay bath over flow stream (SR1) to the pre-mixing tank (denoted as SK1) is analysed. Wastewater from the bottom flow (SR2) is not considered here as it is highly contaminated with impurities (mainly suspended solid) from the cracked mixture. In Scheme 2, the bottom flow of the clay bath (SR2) is purified in a filtration unit for further recovery of fresh water and clay (shown in the box in Fig. 9). In order to avoid accumulation of impurities in the clay bath, 5% of the wastewater is purged from both the over flow and bottom flow streams. Note that the purge portion of both sources is excluded from the available source flowrate for recovery. The limiting data and the property operators are summarised in Table 2.

As discussed before, in order to achieve high separation efficiency of the cracked mixture, the slurry in the clay bath should posses a density of 1120 kg/m^3. Thus, density is identified as the most critical property for wastewater recovery. Shelley and El-Halwagi [58] reported the general mixing rule for density as follows:

$$\frac{1}{\bar{\rho}} = \sum_i \frac{x_i}{\rho_i} \tag{16}$$

where $\bar{\rho}$ is the mean density of the mixture; ρ_i is the density of i stream. The property operator for density can be expressed as [58]:

$$\psi(\rho_i) = \frac{1}{\rho_i} \tag{17}$$

As mentioned earlier, automated targeting is based on the principle of cascade analysis [13,17,27,60]. In most cases, the mass [13,17,27] or property load [60] is cascaded downward from lower to higher concentration/operator level when fresh resource is located at the lowest level. There may be also cases when fresh resource is found at the highest level, in which the load cascade is carried out in reverse direction [60]. In the former (majority of the cases), process sinks with mass/operator level lower than the pinch will receive a mixture of sources which supplies mass/property load up to its maximum limit. In contrast, process sinks with mass/operator level higher than the pinch are allowed to receive a mixture of mass/property load that is lower than its maximum allowable permissible load. However, it is not the same for the clay bath system. From Table 2, it is noted that fresh water and clay posses the highest and lowest property operator, respectively. This means that they are located at the first and last levels in the property interval diagram. Hence, this problem is classified as a bilateral property integration case. If a conventional cascade analysis [13,17,27,60] is carried out, only fresh water or clay will be minimised, but not both. To minimise both fresh water and clay, one would have to ensure the load is also maximised for sinks having operator level higher than the pinch. Since the mass/property load is cascaded down the concentration/operator level when fresh resource is located at the lowest level (or vice versa), another cascade needs to be carried out in a reverse order (decreasing order of level) to minimise fresh resource that is located at the highest level. Furthermore, the two cascades will have to be carried out simultaneously in order to minimise both fresh resources. This calls for a new approach presented, where two reverse sets of cascades are carried out simultaneously. Note that each set of cascade consists of both material flowrate and property load cascades, respectively. In the first set of cascades, the property operators are arranged in an ascending order where fresh water is located at the highest operator level. This set of cascades shall be termed as the *superior cascade* (referring to the fresh resource that is found at the superior operator level). In contrast, property operators are arranged in a descending order in the second set of cascades, where fresh clay is located at the highest operator level. This set of cascades is known as the *inferior cascade*.

Since the superior and inferior cascades are optimised simultaneously and the property load is cascaded in two directions, all the process sinks received mass/property load up to its maximum limit. Hence, the accumulated flowrate for wastewater discharge at the final property operator level is not allowed. Thus, in each level where a source exists, a new sink (F_T) is added to allow the waste to be discharged from the same level to avoid accumulation of wastewater when the net material flowrate (δ_k) is cascaded along the cascades. Thus, Eq. (3) is modified for this property operator level as follows:

$$\delta_k = \delta_{k-1} + \left(\sum_i F_{SRi} - \sum_j F_{SKj} - F_T \right)_k \tag{18}$$

Superior cascade may be carried out following the above-mentioned procedure. In contrast, Eq. (4) is modified for the inferior cascade so that the difference between the property levels k and $k+1$ is set as positive. This ensures a feasible property load cascade

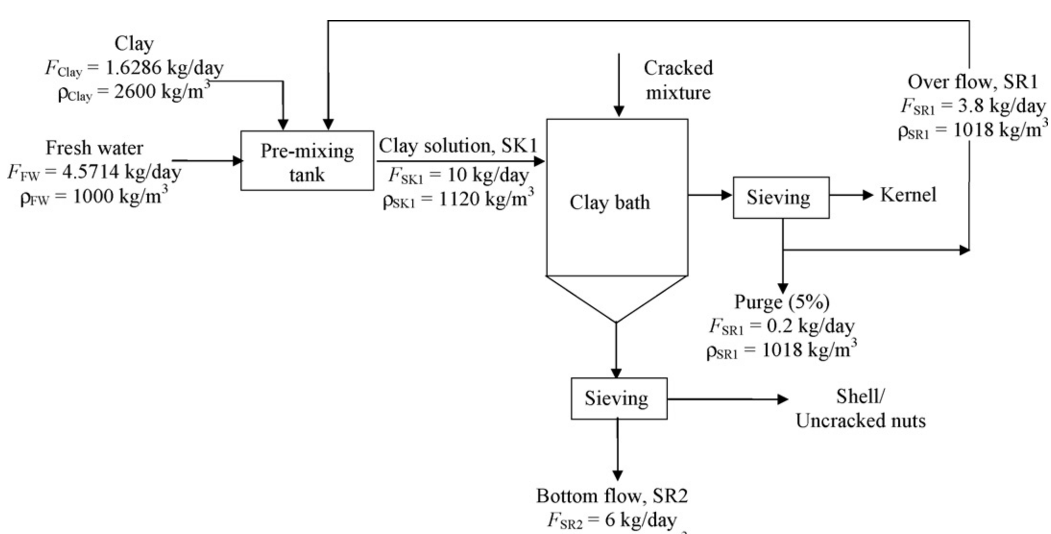

Fig. 11. Optimum design of clay bath system with water recycling (Scheme 1).

to be generated.

$$\varepsilon_k = \varepsilon_{k-1} + \delta_k(\Psi_k - \Psi_{k+1}) \quad (19)$$

Solving the LP model of Eq. (6) subject to Eqs. (3)–(5) for superior cascade, and Eqs. (3), (5) and (19) for inferior cascade simultaneously yield the solution as in Fig. 10(a) and (b). As shown, fresh water (F_{FR1}) and clay (F_{FR2}) flowrates are targeted as 4.5714 kg/day and 1.6286 kg/day, respectively. Fig. 11 shows the design of clay bath with recovery of Scheme 1. Note that SR1 is fully recycled into the clay bath.

The second wastewater recovery scheme with regeneration unit is next illustrated. A filtration separation system is introduced in this scheme to purify the clay bath bottom stream for further recovery. Ng [65] termed a regeneration process with two outlet streams

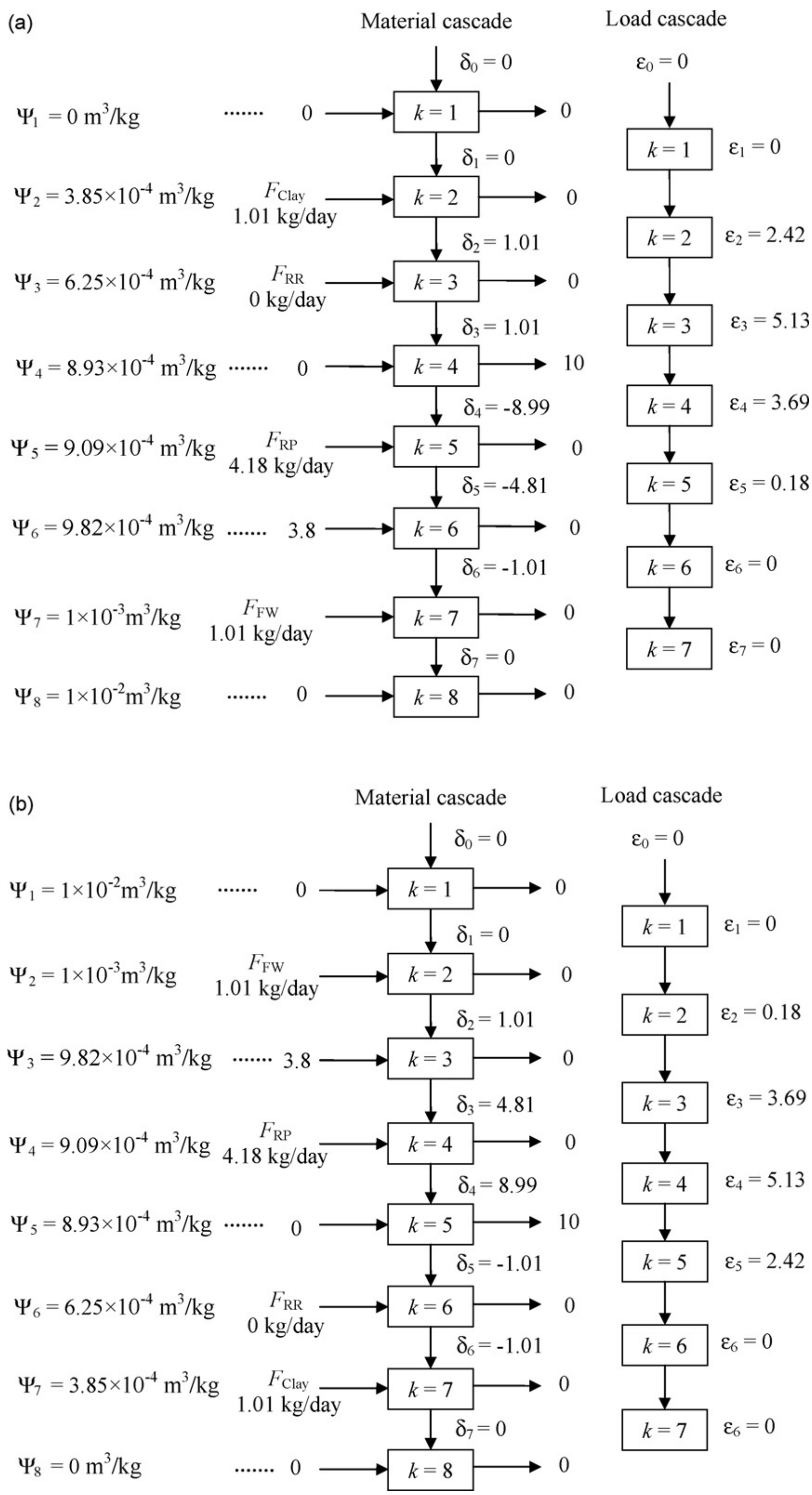

Fig. 12. (a) Superior cascade for Example 2 (Scheme 2). (b) Inferior cascade for Example 2 (Scheme 2).

as *partitioning regeneration* system, where a feed stream is separated into two outlet streams of different quality, i.e. a higher quality product stream and a lower quality reject stream. In the case of Scheme 2, both purified (RP) and reject streams (RR) from the filtration unit are allowed to be recycled to the clay bath, but not simultaneously. This is to avoid remixing of the purified and reject streams. Hence, Eq. (20) is added in the optimisation model:

$$F_{RP} \times F_{RR} = 0 \tag{20}$$

where F_{RP} and F_{RR} refer to the flowrate of the purified and reject streams. However, including this bilinear constraint converts the problem into a non-linear model. In addition, two extra property operator levels (9.09×10^{-4} m^3/kg and 6.25×10^{-4} m^3/kg for purified and reject stream, respectively) are to be added in superior and inferior cascades, as shown in Fig. 12(a) and (b), respectively.

In this work, it is assumed that both outlet streams from the filtration system to have fixed density (as listed in Table 2). It is further assumed no water loss or generation are found in the filtration system. To include the regeneration model into the automated targeting framework, the flowrate (Eq. (21)) and property load balances (Eq. (22)) are added:

$$F_{RWW} = F_{RP} + F_{RR} \tag{21}$$

$$F_{RWW}\,\psi(\rho_{RWW}) = F_{RP}\,\psi(\rho_{RP}) + F_{RR}\,\psi(\rho_{RR}) \tag{22}$$

where $\psi(\rho_{RWW})$, $\psi(\rho_{RP})$ and $\psi(\rho_{RR})$ are the density operators of the wastewater that is sent for regeneration, purified stream and reject stream, respectively. Note that when considering Eqs. (20) and (21) simultaneously, either F_{RP} or F_{RR} will be forced to become zero, which leaves the other term to become the treated wastewater flowrate (F_{RWW}) in Eq. (21).

Generally, the operating cost of regeneration increases proportionally with the wastewater flowrate entering the filtration system. Hence, in order to synthesise a cost effective water recovery system, it is necessary to minimise the total operating costs of the fresh materials and the regeneration flowrates. The TOC function in this case resembles that of Eq. (8), and given as follows:

$$\text{TOC} = A\,F_{FW} + B\,F_{Clay} + C\,F_{RWW} \tag{23}$$

where F_{FW}, F_{Clay} and F_{RWW} are the flowrates of the fresh water, clay and regeneration, respectively; while *A*, *B* and *C* reflect the unit cost for each of these sources, which may be determined from historical data or estimation. In this case it is assumed that *A*, *B* and *C* to bare a value of \$1.00/kg, \$2.00/kg and \$0.05/kg, respectively.

Solving the NLP model with the objective function in Eq. (23) (subject to Eqs. (3)–(5) of superior and Eqs. (3), (5) and (19) of inferior cascades, and Eqs. (20)–(22)) yields the result as shown in Fig. 12(a) and (b). As shown in Fig. 12(a) and (b), the fresh water (F_{FW}) and fresh clay (F_{Clay}) consumptions are both targeted as 1.01 kg/day. The total annual operating cost of the clay bath is determined as \$1094 (annual operation is assumed as 330 days), and the optimum design of clay bath with clay recovery (Scheme 2) is shown in Fig. 13. As shown, 5.70 kg/day (=4.18 kg/day + 1.52 kg/day) of bottom flow (SR2), F_{RWW} is being regenerated by the filter and 5% of bottom flow is discharged. It is noted that the purified stream (RP) and over flow (SR1) are fully recycled into clay bath in this scheme. Note that the same results for Schemes 1 and 2 can also be found with a superstructural optimisation model (e.g. El-Halwagi [2]).

9. Placement of pre-treatment system

Pre-treatment system is commonly used in the process industries to treat the fresh material into higher quality, before it may be used in the process. For example, municipal fresh water is treated with pre-treatment system to generate ultra pure water (UPW) for the use in the semiconductor industry. Generally, water pre-treatment system consists of three main elements which are ultra-filtration (UF), reverse osmosis (RO) and deionisation (DI). UF is used to retain the solute of high molecular weight contaminants in the municipal fresh water; while RO and DI processes are used to remove the low-molecular weight ions in the water content. Most of the process industries treat the reject streams from the

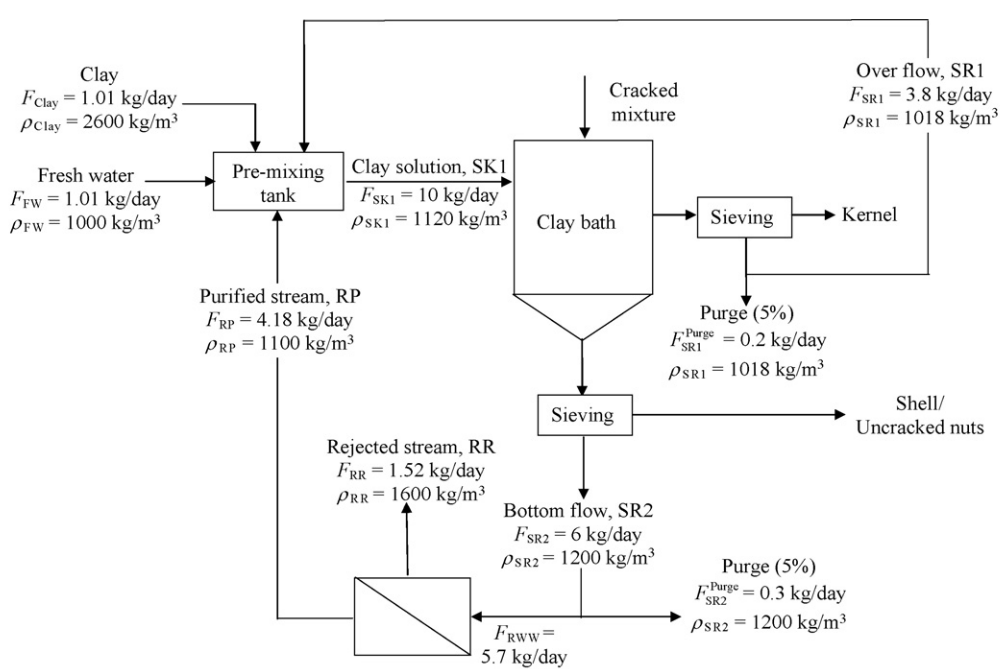

Fig. 13. Optimum design of clay bath system with regeneration (Scheme 2).

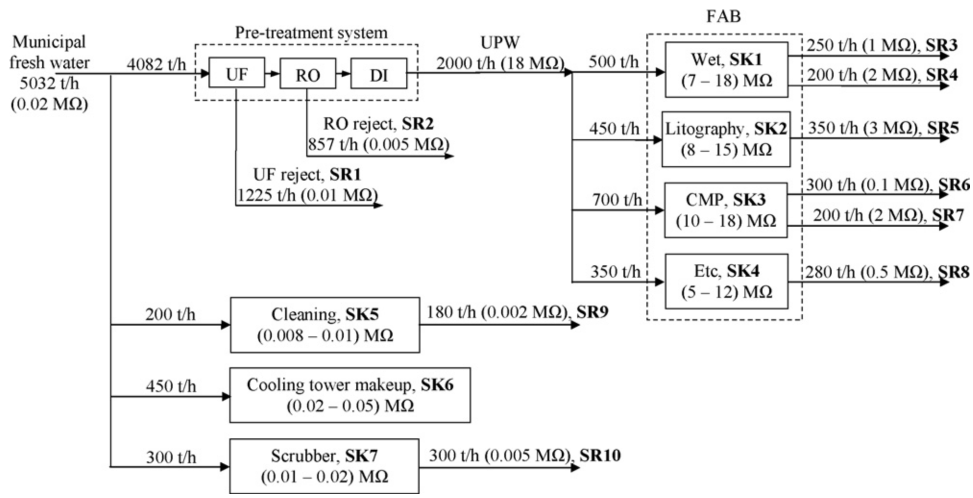

Fig. 14. Schematic diagram for wafer fabrication process.

pre-treatment system as wastewater. However, as will be shown in the later section of the paper, the reject streams can actually be considered for recovery in order to further reduce effluent from the plant.

In this work, the interaction of a pre-treatment system with RCN is analysed. Note that no work has been reported to date for the analysis of this interaction in the open literature. Example 3 is used to illustrate the proposed method.

10. Example 3

An industrial wafer fabrication process is used to illustrate the application of the automated targeting technique for a RCN with pre-treatment system. In this example, the pre-treatment system is used to generate UPW to fulfil the process requirements. It is assumed that 70% of the inlet flowrate of UF to pass through the membrane as permeate; while, 30% of the flowrate is rejected as wastewater with constant water quality. The same assumption applies for the RO membrane. In order to reduce fresh water consumption, the recovery of reject stream from the pre-treatment system should be considered. It is notable that the flowrate of the reject stream is dependent on the amount of water that is fed to the pre-treatment system. This dependency enables the interactions to be explored between the pre-treatment system and the water network.

Fig. 14 shows a schematic diagram for a wafer fabrication process with a water pre-treatment system. As shown in Fig. 14, there are four sections in the wafer fabrication (FAB) process that require UPW supply, denoted as "Wet," "Lithography," "CMP" (i.e. combined chemical and mechanical processing) and "etc." (miscellaneous processes). Besides, cleaning, cooling tower makeup and scrubber as well as pre-treatment system necessitate an external supply of municipal fresh water. Note that the Wet and CMP sections generate two wastewater streams with different water quality. Besides, ten water sources may be considered for water recovery. In this case study, the most significant water quality factor was determined to be resistivity (R), which constitutes an index of the total ionic con-

Table 3
Limiting data for Example 3.

Process	Flowrate (t/h)	Resistivity, R (MΩ)		Property operator, Ψ (MΩ^{-1})	
		Lower bound	Upper bound	Lower bound	Upper bound
Sink					
Wet (SK1)	500	7	18	0.1429	0.0556
Litography (SK2)	450	8	15	0.1250	0.0667
CMP (SK3)	700	10	18	0.1000	0.0556
Etc. (SK4)	350	5	12	0.2000	0.0833
Cleaning (SK5)	200	0.008	0.01	125	100
Cooling tower makeup (SK6)	450	0.02	0.05	50	20
Scrubber (SK7)	300	0.01	0.02	100	50
Source					
UF reject (SR1)	30% inlet flowrate of UF	0.01		100	
RO reject (SR2)	30% inlet flowrate of RO	0.005		200	
Wet I (SR3)	250	1		1	
Wet II (SR4)	200	2		0.5	
Litography (SR5)	350	3		0.3333	
CMP I (SR6)	300	0.1		10	
CMP II (SR7)	200	2		0.5	
Etc. (SR8)	280	0.5		2	
Cleaning (SR9)	180	0.002		500	
Scrubber (SR10)	300	0.005		200	
Ultra pure water (UPW)	To be determined	18		0.0556	
Municipal fresh water (FW)	To be determined	0.02		50	

tent of aqueous streams. The general mixing rule for resistivity is given as [2]:

$$\frac{1}{\bar{R}} = \sum_i \frac{x_i}{R_i} \quad (24)$$

Note that the property operator for resistivity is defined as the inverse of resistivity (R^{-1}), such that the lowest resistivity also corresponds to the lowest quality level. Table 3 summarises the pertinent data for the sinks and sources. In this case study, the lower bounds of the resistivity are selected as the limiting property for process sink when water recovery scheme is considered, because these lower bounds correspond to the lowest stream quality that can be tolerated by the processes, and thus maximises the potential for water reuse and recycling.

Since the reject streams from the UF and RO systems are dependent on the inlet flowrate of municipal fresh water into pre-treatment system, equations below are also included in the optimisation model:

$$F_{\mathrm{In}}^{\mathrm{UF}} = F_{\mathrm{P}}^{\mathrm{UF}} + F_{\mathrm{R}}^{\mathrm{UF}} \quad (25)$$

$$F_{\mathrm{In}}^{\mathrm{RO}} = F_{\mathrm{P}}^{\mathrm{RO}} + F_{\mathrm{R}}^{\mathrm{RO}} \quad (26)$$

where $F_{\mathrm{In}}^{\mathrm{UF}}$ and $F_{\mathrm{In}}^{\mathrm{RO}}$ are the inlet flowrate to the UF and RO system, respectively. Meanwhile, $F_{\mathrm{P}}^{\mathrm{UF}}$ and $F_{\mathrm{R}}^{\mathrm{UF}}$ represent permeate and reject flowrates for the UF system; $F_{\mathrm{P}}^{\mathrm{RO}}$ and $F_{\mathrm{R}}^{\mathrm{RO}}$ are the flowrate of permeate and reject streams for the RO system. Since all the permeate flowrate of UF and RO systems is directly sent to next treatment unit to generate UPW; therefore, $F_{\mathrm{In}}^{\mathrm{RO}}$ is equivalent to $F_{\mathrm{P}}^{\mathrm{UF}}$, and the UPW flowrate ($F_{\mathrm{UPW}}$) is same as $F_{\mathrm{P}}^{\mathrm{RO}}$.

In addition, as discussed previously, 30% of the inlet flowrate for UF and RO systems is rejected as wastewater; thus, Eqs. (27) and

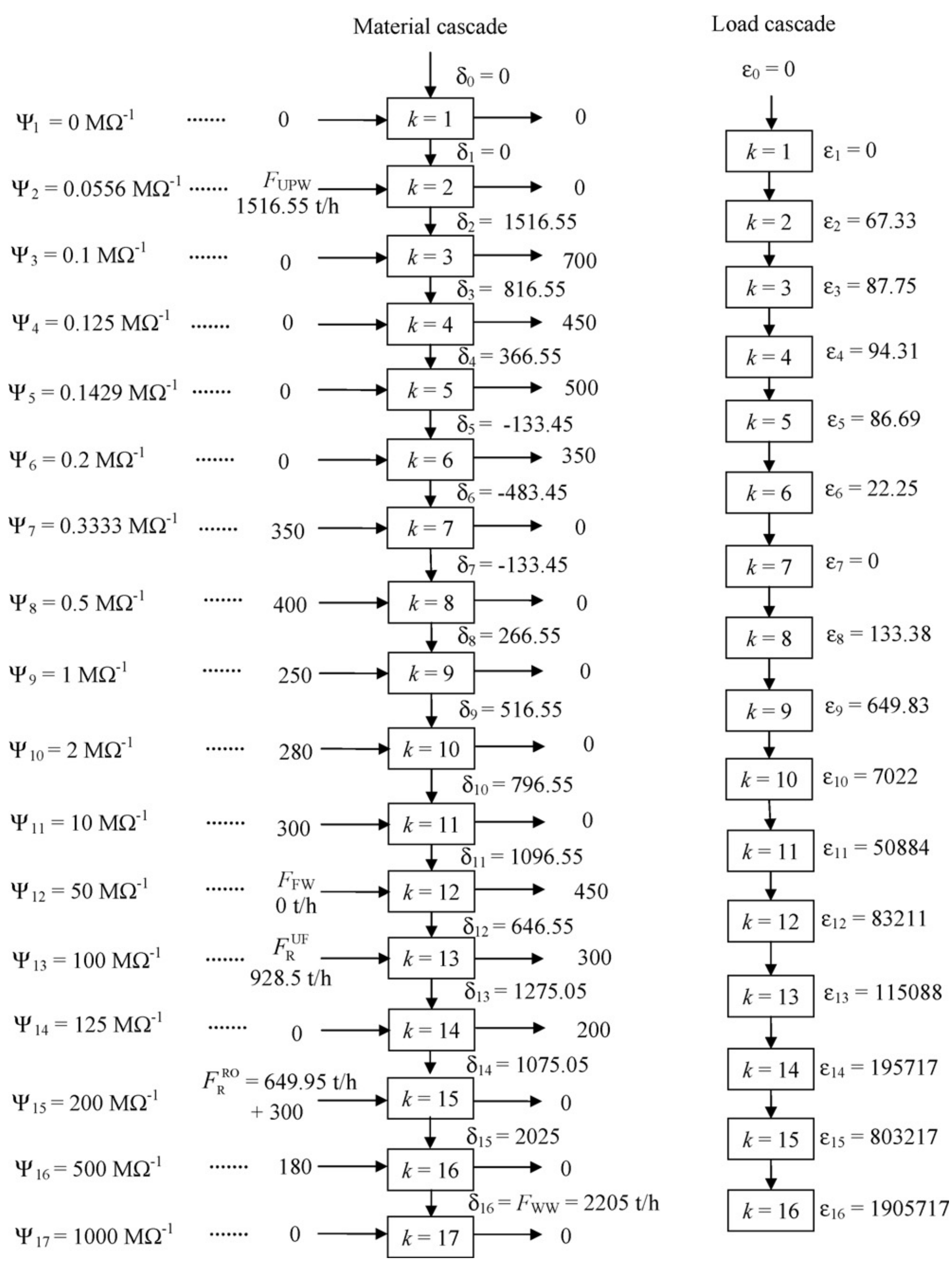

Fig. 15. PCD for Example 3.

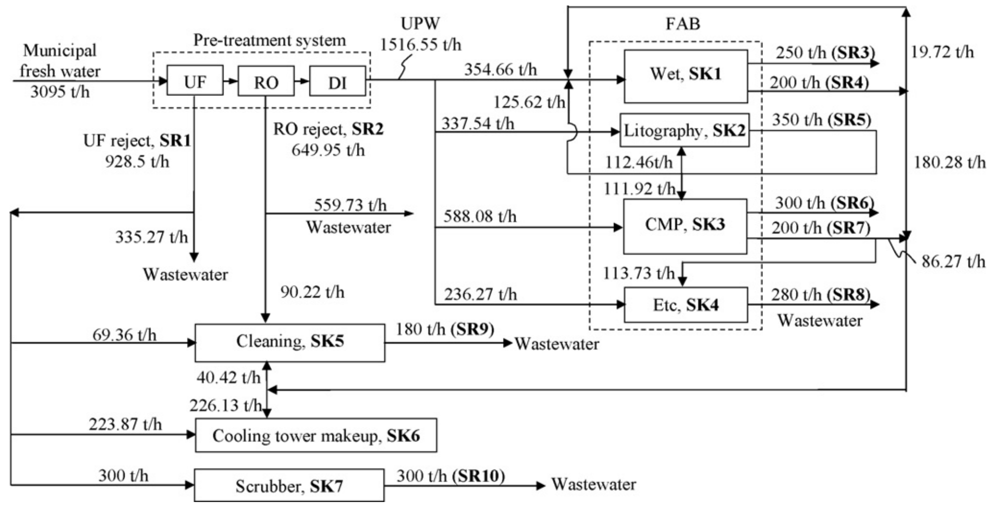

Fig. 16. Optimal water recovery scheme for wafer fabrication process (Example 3).

(28) are also included in the optimisation model:

$$F_R^{UF} = 0.3 \times F_{In}^{UF} \quad (27)$$

$$F_R^{RO} = 0.3 \times F_{In}^{RO} \quad (28)$$

Following the proposed automated targeting technique, the optimisation model is solved to minimise the overall municipal fresh water (Eq. (7)), i.e. fresh water for pre-treatment (F_{In}^{UF}) and fresh water for other processes (SK5–SK7), subject to the constraints in Eqs. (3)–(5), and Eqs. (24)–(28). The PCD for Example 3 is generated in Fig. 15. Note that the total municipal fresh water and wastewater flowrates are targeted as 3095 t/h (=928.5 t/h + 649.95 t/h + 1516.55 t/h) and 2205 t/h, respectively. Note that all municipal water is passed through the pre-treatment system to form UPW. The optimal water recovery scheme for Example 3 is showed in Fig. 16, obtained via the nearest neighbour algorithm [14].

11. Conclusion

This work presents the extension of the automated targeting technique to establish the resource targets within a property integration framework, which is essential in process applications wherein stream quality depends on functional properties, as opposed to concentrations of specific contaminants. The automated targeting technique combines the advantages of both insight-based and mathematical optimisation approaches. However, the approach developed is more flexible than conventional pinch analysis techniques, since process modifications or design restrictions can be readily integrated within the optimisation model. Automated targeting for property-based RCN synthesis that involved process modification for further material recovery is presented. In addition, interaction of pre-treatment system with water recovery network is also analysed in this work. Finally, a new approach for the bilateral property integration problem is presented where two reverse sets of cascades are preformed simultaneously to minimise the fresh resources with lowest and highest property operators at once. Literature and industrial cases were used to illustrate the proposed approach. Further work is still required to extend the dual cascade approach to more complex bilateral property integration problems; for example, in cases when multiple fresh resources exist at different levels in the property operator scale.

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