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Industrial site water exchange network synthesis considering multiple quality constraints and water headers



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ABSTRACT

This work aims to extend the previous Pinch Analysis framework to the industrial site material recycling network with site headers synthesis from single quality to multiple qualities. The analysis provides guided resources management strategy in any eco-industrial park to reduce the reliance on raw resources that are extracted from the environment. The Pinch Point(s) are first identified for the overall network using the Material Recovery Pinch Diagram for all the qualities. The guideline for the cross-plant material sources transfer is then built upon the concept of the Pinch Point(s) for all the qualities to minimise the cross-plant source transfer or a number of connections. An iterative header targeting framework is then proposed to determine the flowrates and the qualities of the headers. Two case studies, which have single and multiple qualities Total Site water recycling network, are used to demonstrate the proposed framework, comparing results obtained using direct integration and centralised headers. The single quality case results in 4.1% lower fresh resource intake compared to without cross-transfer, while the multiple qualities case could have 5.3% lower fresh resources for two and three plants scenarios. This framework provides a proper analysis of the problem, which allows users to gain insights on the effective cross-plant source transfer schemes with headers constraint by resource qualities.

1. Introduction

Escalated industry development has significantly increased global consumption and wastewater disposal. It is found that in the next three decades, global water consumption is expected to increase by 55% (OECD, 2021), which is an alarming issue. A tactical approach is needed to allow practitioners to strategically plan for water recycling rate improvement while reducing the discharge of wastewater.

Process Integration tool, namely Pinch Analysis, is a matured method in the past decades and applied in various industries for wastewater or freshwater minimisation. The pioneering concept was introduced by Wang and Smith (1994). This method uses a concentration-based representation for the water cascade, presenting a close analogy with the Heat Cascade from Heat Integration (Linnhoff et al., 1994). At a later stage, El-Halwagi et al. (2003) has mentioned that most industries contain material recycling issues rather than impurities exchange problems. They introduced a Material Recovery Pinch Diagram for water recycling problem represented in source-sink formulation, which effectively determines the Pinch Point and target for minimum fresh resource or wasted sources. Cascade analysis is then developed by Manan et al. (2004) based upon a similar concept and accurately locating the Pinch Point numerically. Bandyopadhyay (2006) then proposed the similar concept of maximising sources recycling to reduce waste, instead of focusing just on minimising fresh resources. The recent study by Chin et al. (2021c) demonstrates the optimal water recycling strategy involving multiple qualities to satisfy the sink's quality limit as much as possible, i.e. reaching Pinch Points for all the sinks, provided if the source arrangement sequence is conflicting. The overall development was detailed in a handbook by Klemeš et al. (2018).

Concerning the resource conservation problem in Total Site, a hierarchical method is presented by Liao et al. (2007), in which the fresh resources are targeted first, and network design with minimum cross-plant connections are formulated and solved with a mathematical approach. By analysing the Composite Curves representation of individual plants, Chew et al. (2010a) proposed an unassisted integration scheme that focuses on direct cross-plant transfer that guarantees resources reduction. Chew et al. (2010b) later proposed assisted integration scheme, where requires a mutual transfer in order to reduce the fresh resource. A recent study by Chin et al. (2021b) has extended the previous analyses and proposed more cross-plant transfer schemes. Several extensions on the water industrial park studies can be found. Lim and Park (2010) applied life cycle assessment to determine the economic and environmental feasibilities of a water industrial park. Boix et al. (2012) incorporated wastewater regeneration options in the Total Site.

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Alnouri et al. (2014) considered the piping merging with concerns of limited space availability, and Jiang et al. (2019) explored different stations that generate water resources as utilities for the system. Multi-period studies are done by Liu et al. (2018), who considered production expansion with predicted variations on the system, and Ramin et al. (2021), who determine the optimal incremental system design along with different treatment units specifically for the Kenya region. Aguilar-Oropeza et al. (2019) studied the acceptability of the network system in the water industrial park by proposing a strategy to generate a set of solutions with trading-off objectives. A recent study by Dong et al. (2021) assessed the grey water footprint of an industrial site located in Guangzhou, China. They identified phosphorus and nitrogen as the critical pollutants for water shortage issues and suggested the importance of recycling wastewater and preserving the qualities of natural water bodies. Cruz-Avilés and Munguía-López (2021) incorporated fairness in their approach in designing water networks in eco-industrial parks. Chin et al. (2021a) later applied the cooperative game approach in fair allocating the government subsidy to the stakeholders and evaluating the taxation policy using a single quality problem. Mentioned studies are focused on a different extension to the Total Site or water industrial park study, which can be solved with a mathematical approach.

Water Integration problems originating from superstructure optimisation can be difficult to implement due to piping complexity and low operability. Feng and Seider (2001) first proposed the water header concept that allows internal water main for water network. The water main allows easier controllability to the water sources with less complexity. Wang et al. (2003) later extended the concept to multiple contaminants, and Cao et al. (2004) applied for water regeneration as well. However, the number and quality of the headers/mains are usually pre-determined. A water heater/main can be modelled as a mixer for various sources and act as a splitter to distribute the sources to the demands. Too few headers would lead to over-mixing of the sources and deteriorate the quality of the sources, which result in more fresh resource requirements. Too many headers would result in too high investment cost and high complexity, which is the opposite of the purpose of the water mains design.

Chen et al. (2010) provided a non-linear optimisation model for water recycling in an industrial park considering the water header concept. Fadzil et al. (2018) utilised the Pinch Approach in designing centralised water reuse headers for a single contaminant. Their approach considers all sources available in all plants to be mixed in the pre-determined headers. The solutions obtained can cause an unnecessary transfer to the headers, causing more pumping power. A systematic method for determining the optimal number of headers with optimal qualities should be defined. Chin et al. (2021d) applied the Composite Curves concept in targeting the properties of the internal header: a number of headers, header sources qualities and flowrates of header sources in a single step. The method is applicable for a single quality problem. Chin et al. (2021b) applied this concept for the Total Site problem. Chin et al. (2021e) also proposed a water main design with a mathematical approach. However, they proposed internal headers targeting for multiple qualities problem, but not effective for Total Site problem with the minimal cross-plant transfer. The Composite Curves for multiple qualities should be critically analysed to identify the optimal cross-plant transfer strategies that reflect the reality.

Few studies are focused on analysing the system strategically to reduce fresh resource constraints by resources quality, which enables the users to plan for the system design. Although Chew et al. (2010a) has analysed the problem, and Chin et al. (2021b) extended the analysis, the multiple qualities problem still poses a difficulty of using the Pinch-based concepts for the site-level recycling problem. The Pinch-based concept allows identification of the feasible cross-plant source transfer aided with visualisation tools while ensuring the fresh resources are minimised. This provides physical insights on the optimal resource recycling and cross-plant sources transferring strategies and can be complemented with other approaches (such as Mathematical Programming) to have better-informed resource management solutions. The problem of site-level headers design with Pinch-based concept should be extended to multiple qualities so that the users can identify the centralised headers with minimal cross-plant transfer easily.

As such, this study proposes a graphical analysis for the design of Total Site Water Integration networks with minimal cross-plant transfer and water header, considering multiple qualities. The main difference between this work and the previous studies is an implementation of enhanced Pinch Analysis concepts in identifying the minimal cross-plant transfer schemes for multiple qualities while guaranteeing minimal fresh resources requirements. The novelties of this study are:

- (i) Provide guided strategies in minimising the number of crossplant source transfers for multiple qualities using the extended Pinch-based concept. The graphical visualisation with Pinch approach provides an interface or the users to understand various feasible cross-plant transfer schemes, reducing the number of connections or source transfer
- (ii) The parameters for site-level headers or resource storages, including the number of headers or quality of header sources, are determined with the minimal cross-plant sources and minimal fresh resources

2. Problem statement

This work emphasises the material conservation network problem in the Total Site level constrained by multiple qualities, which is the problem class of Mass Integration. The quality indicators range from contamination levels to other physical properties that can be measured and identified by mixing rules. The problem class covers any material types, ranging from solid waste, CO₂, hydrogen or water. Each industrial plant has specific demands/sinks that can be fulfilled by reusing the supplies/sources generated from either the same plant or other plants. The unwanted materials produced from the industrial plants or sites pose as valuable secondary resources that can be recycled to reduce the reliance on fresh resources. The fresh resources can be supplemented when the recycling potential of all the sources have been exploited. For site-level integration, the cross-plant sources flow between plants also should be minimised to reduce the pumping cost or the number of transfers to be optimised to reduce the piping connection. This work also considers the material headers/mains synthesis into the problem, which allows easier resource management. The number of headers, sources flow and qualities inside the header is the main variables to be determined. Fig. 1 shows the illustration of the problem.

The main problems to be solved are:

- (i) What are the optimum strategies that can be obtained from the solutions of Pinch Analysis in minimising the cross-plant source transfer?
- (ii) Given the minimum cross-plant sources (number of connection/ flowrates), what are the optimum number or qualities of the header sources for the regional system?

3. Concepts and methodology

This section covers the explanation of the concept for targeting and designing the Total Site material headers/mains with the Pinch-based approach. Section 3.1 first explains the Pinch-based concepts in sources allocation using Composite Curves for single quality. Section 3.2 then extends the Pinch Points definition to multiple qualities and their relation with sources allocation. Section 3.3 denotes the cross-plant source transfer using the Pinch-based concepts, and Section 3.4 covers the headers targeting framework for multiple qualities problems.



Fig. 1. Demonstration of Site-level water recycling network with water headers.

3.1. Pinch principles in sources allocation - single quality

For Mass-Based Integration within an industrial plant, the wasted material sources generated by each unit operation can be recycled to material sinks of other unit operations. El-Halwagi et al. (2003) proposed a graphical framework called Material Recovery Pinch Diagram (an adaptation is shown in Fig. 2a) to target the maximum recycling of the material sources and minimum fresh resource intake for a certain process, and Prakash and Shenoy (2004) introduced the concept as well and applied to fixed flow and fixed load operations. It is a diagram that has the material quality load (e.g. contaminant load for water) on the y-axis and flowrates of the material streams on the x-axis. The material sinks are arranged with descending order of the quality or ascending order of the contaminant concentrations in the water case (increasing gradient). The Sink Composite Curve (CC) is constructed by stacking all the segments of the sinks in the arranged order, where a segment represents a sink. The material sources are also usually arranged in a similar order. This arrangement tells the core principles in the allocation of the sources:

- (i) Demand/sink that has the highest quality (lowest contamination limit for water case) is to be fulfilled first, followed by the next highest quality.
- (ii) Supply/source that has the highest quality should be utilised first, followed by the next highest quality

For a pure fresh resource, the Source CC has to be shifted horizontally

to the right (from the origin point) until it is entirely below the Sink CC. This signifies that the limits of the qualities for all the sinks are satisfied. Fig. 2a shows the demonstration of a typical CC. Focusing on the region around the Pinch Point: the Pinch Point divides the network into two regions Below and Above the Pinch. The sinks Below the Pinch Point (or to the left of the Pinch) require fresh resource supply as they are constrained by the sources' quality, while the sinks Above the Pinch Point (or to the right of the Pinch) are not constrained by the sources' quality and can be fulfilled only by the available sources. The Below Pinch region is denoted as the High-Quality Region (HQR), while the Above Pinch Region is labelled as the Low-Quality Region (LQR).

For a single quality problem, the source arrangement Below or Above the Pinch Regions can be swapped within their own regions only without changing the minimum fresh resource intake. Fig. 2b shows that Source 2 and Source 1 are swapped with their position. Instead of prioritising Source 1, Source 2 is used up first before Source 1 during the source allocation. This prioritising sequence changes the fresh resource requirements for each sink, but it does not alter the overall fresh resource requirement for the whole network. This is due to the Plus-Minus Principles for the fresh resource requirement for each sink. A similar arrangement can also achieve the same outcome by just swapping part of Source 2 - Fig. 2c, or reversing the order of the arrangement of the source in the high-quality region - Fig. 2d.

However, the arrangement of sources should be made so that the allocation could fully fulfil the contamination limit for all the sinks. Otherwise, it may incur additional requirements of fresh resources, as shown in Fig. 3. If one of the sinks in the High-Quality Region has not



Fig. 2. Feasible CC representations with different source arrangement in the HQR region (Below Pinch) provided if all quality limits of sinks in HQR are reached (a) Ascending order of sources (b) Swapping position of Source 1 and 2 (c) Splitting part of the sources and arrange them in different positions (d) Descending order of sources. HQR: High-Quality Region, LQR: Low-Quality Region, adapted from El-Halwagi et al. (2003).



Fig. 3. (a) A typical Composite Curves with an arrangement based on descending order of quality (b) Source 2 is swapped with Source 1, causing violation with the arrangement.

fulfilled the contamination limit, this means the high-quality sources is actually wasted for the lower quality sink and cause the overall fresh resource to be increased. This can be observed in the downward shift of Sink CC in Fig. 3, where the real quality limit of the sink is cascaded to the next sink. This observation is crucial when defining the Pinch Points for multiple qualities problem.

3.2. Defining Pinch Points in multiple qualities problem

The Pinch Points for the multiple qualities problem should be first identified to understand the characteristic of the optimal synthesis Total Site Material Integration problem with multiple qualities. The fresh resource targeting procedure, using the Composite Curves for multiple contaminants, is more complicated than the case of a single contaminant. Based on Chin et al. (2021c), it first requires determining the limiting contaminants for each sink so that the sources allocation sequence can be identified. The individual source-to-sink allocation is then performed with CCs with the arrangement of sources based on the limiting contaminant of each sink and needs to check which contaminants limits are not fulfilled. Those that are not satisfied require some shifting in the Sink CC (Fig. 4). In Fig. 4a, which considers Sink 1 only, the limit for quality B is not reached, so the next sink segment should be shifted downward to accommodate the reduced sink load of Sink 1 – see Fig. 4b. It can be seen that a 'pseudo' Pinch at the Quality B for Sink 2.

Based on the results from Chin et al. (2021c), the optimal source allocation depends on the qualities of the source streams. If all the sources are non-conflicting in their qualities, i.e. the source arrangement based on Quality A is the same as Quality B, then the source allocation

based on the limiting quality/contaminant could already ensure minimal fresh resource requirements. However, if all the sources are conflicting in the source arrangement, then the arrangement or allocation of the source to the sinks should ensure all the qualities limits of the sinks should be satisfied as much as possible. A demonstration of a simple two qualities problem with conflicting source arrangement is shown in Fig. 5. The readers can refer to Chin et al. (2021c) for a full demonstration of the optimal source allocation (network design) with Pinch-based concepts. Different approaches such as Mathematical Programming, Water Source Diagram (Calixto et al., 2020) or concentration potential methods (Liu et al., 2009) can be used to determine the source allocation as well. It is required to first identify the allocation of the ideal sources that ensure minimal fresh resources intake to define the Pinch Points for the multiple qualities problem.

After the exact source allocation is performed, Composite Curves can be drawn for the multiple qualities to determine the Pinch Point(s). Unlike a single quality problem, a Pinch Point can be formed for one quality but not necessary for the others. This is shown in Fig. 6, where only the Pinch Point is formed at the limiting quality A, but not at the other quality B. In this case, Source 2 is the Pinch-Causing source for quality A, but none is for B. Ideally, this process or plant could receive any sources that have lower quality than Source 2 for Quality A and no limits on Quality B as long as the sinks' limit is not violated.

For the case of if Pinch is also observed in another Quality B - Fig. 7, the source which has the lowest quality in the below Pinch region should be the Pinch-causing source. For example, Source 2 is the Pinch-Causing source for Quality A, and Source 1 is the Pinch-causing source for Quality B as it has lower quality than Source 2 in terms of Quality B.



Fig. 4. (a) Pinch point at Sink 1 for Quality A but not Quality B (b) 'Pseudo' Pinch at Sink 2 for Quality B.



Fig. 5. Sequential source allocation with a developed methodology for multiple contaminants, adapted from Chin et al. (2021c). Pinch must form at the limiting quality (A) where sources are arranged in ascending order.



Pinch Points = $\{A, B\} = \{C_{SR2A}, \infty\}$

Fig. 6. Pinch Points for limiting Quality A, but not for non-limiting Quality B.





Fig. 7. Pinch Points for limiting Quality A and for non-limiting Quality B.

Note that in fact, in Fig. 7, the Sources CC is not violating the Pinch Concept as it intersects with Sink CC. This is due to the 'Polygon' rules where it forms a triangle shape with Sink CC, indicating the limit for Sink is still satisfied without violating the limit. The explanation can be found in Chin et al. (2021c). If there are available sources from other

plants, the source which has better Quality A than Source 2 and better Quality B than Source 1 can be used so that the fresh resources can be reduced further.

However, for a problem with Sink CC that is shifted vertically, the definition of Pinch Points are slightly different. If a Pinch is observed

around shifted Sink CC, the Pinch Point is not the real Pinch Point but is just a 'pseudo' Pinch Point. This is because the quality limits for one of the sink is not satisfied, and in fact, any sources from other plants can be used to fulfil the limit. This is shown in Fig. 8, where the Pinch-Causing source is Source 2 for Quality A when for Quality B, there are no Pinch-Causing sources.

3.3. Minimal cross-plant transfer schemes

3.3.1. Single quality

The Composite Curves tells the information on how the cross-plant transfer can be performed to ensure the fresh resources can be further reduced. Chin et al. (2021b) analysed various possible options of cross-plant transfer schemes and recommended three strategies:

- (a) Scheme 1: Transfer of sources from a Low-Quality Region (LQR) of one plant to another plant's High-Quality Region (HQR)
- (b) Scheme 2: Transfer of sources from HQR of one plant to another plant's LQR, followed by at least one Scheme 1.
- (c) Scheme 3: Transfer of sources from LQR of one plant to another plant's LQR, followed by at least one Scheme 1.

Fig. 9 shows the demonstration of the cross-transfer scheme where the source of one plant from the LQR into another plant's HQR. This is feasible when the receiver plant has Pinch Point higher than the Site Pinch Point (lower quality), and the supplier plant has Pinch Point lower than the Site Pinch Point (higher quality). In this example, Plant B has sources in the LQR but has better quality than the Site Pinch Point and can be used to replace sources with quality than the Site Pinch Point in Plant A. This potentially could lower the Pinch Point in Plant A so that its Pinch Point could reach the Site Pinch Point.

Another scheme is when the transfer of source in the HQR of one plant to LQR of another plant is possible, as shown in Fig. 10. In this demonstration, the Pinch-causing source in Plant B is actually wasted in the LQR sinks since the Pinch Point in Plant B is lower than Site Pinch Point. Unlike in Fig. 9, the transfer is from exactly the Point Point in Plant B instead of above the Pinch Point as compared to Scheme 1. In exchange, the HQR source in Plant A, which has worst quality than the Site Pinch Point, can be used to replace the LQR Pinch-causing source in Plant B. Note that the supplier Plant A can send any source which has quality lower than the plant's Pinch Point but higher than the Site Pinch Point. Scheme 3 also follows the same demonstration in Fig. 10. In this case, the supplier Plant A should send the Pinch-causing source (source at the Pinch Point) in the LQR region to the receiver Plant B LQR. Note that for these two schemes, there is a transfer from LQR to HQR (Plant B to Plant A), which allows the reduction of the flows of fresh resources and wasted sources.

In fact, any other cross-plant sources exchanges are possible but may

not be as effective and could incur more unnecessary transfers that cost more. For example, the supplier plant can give up part of their sources in the HQR to send to the receiver plant's HQR, but it is ineffective to the overall fresh resource consumption. By observing the transfer schemes, the plants that have the Pinch Point lower than the Site Pinch Point (higher quality) can send out their sources to other plants that have Pinch Points higher than the Site Pinch (lower quality). This guarantees to reduce the overall fresh resource consumption. This observation is applicable to multiple qualities problem as well, which is explained in the next section.

3.3.2. Multiple qualities

The multiple qualities problem can have a similar representation using Composite Curves as well. Each quality has an individual High-Quality Region and Low-Quality Region, as shown in Fig. 11. The Pinch Points of individual plants and the Site Pinch Point(s) can be identified with Composite Curves as explained in Section 3.2. A feasible and effective cross-transfer scheme can be identified in a similar manner.

It has been shown in the previous section that the supplier plants with Pinch Points lower than the Site Pinch Points can transfer their sources to receiver plants with Pinch Points higher than the Site Pinch Points. Fig. 12 shows an example of a feasible transfer scheme (Scheme 1) for the two qualities problem. The supplier plant (Plant B) has Pinch Points lower or equal to the Site Pinch Points for both qualities, and the receiver plant (Plant A) has higher Pinch Points than the Site Pinch Points for both qualities. Note that the Pinch Points are the Real Pinch Points, not the 'Pseudo' Pinch Points.

In the demonstration shown in Fig. 13, it is shown that the receiver and supplier both have Lower Pinch Point for Quality B. In terms of Quality A, Plant B can supply its source from its LQR to Plant A's HQR since Plant A has a Higher Pinch Point than the Site Pinch Point. Since both plants have Lower Pinch Points for Quality B, the transfer can be ineffective for Quality B but effective for Quality A. Since also Plant B has a Lower Pinch Point in Quality B than Plant A, the transfer from Plant B LQR to Plant A HQR is still effective and feasible.

However, in the case where Plant B has a higher Pinch Point in Quality B than the Site Pinch Point - see Fig. 14, the cross-plant transfer of LQR (Plant B) to HQR (Plant A) is actually ineffective, although it is effective in terms of Quality A. The alternative schemes presented in the previous section should be sought out instead. The cross-plant transfer strategies from the single quality representation are applicable to multiple qualities as well, but the transfer should be checked for all qualities. The Pinch Points for multiple qualities are also strongly dependent on the source-to-sink allocation strategy, so it is required that the network design should be known prior to analysing the Composite Curves. To summarise, Table 1 shows the possible transfer schemes between plants that are effective for reducing overall fresh resources.



Pinch Points = $\{A, B\} = \{C_{SR2A}, \infty\}$

Fig. 8. Pinch Points for limiting Quality A, but not for non-limiting Quality B (just 'pseudo' Pinch).



Fig. 9. Plant B send its unused sources (LQR) to Plant A (HQR higher than Site Pinch). Pinch Point for plant B is lower than the Site Pinch Point.



Fig. 10. Plant B send its unused sources (LQR) to Plant A (HQR), and Plant A send its sources at the Pinch Point from LQR (HQR higher than the Site Pinch Point) to Plant B (Pinch Point). Plant A would require another source with quality at the 'Site Pinch' Point.



Fig. 11. Division into High-Quality Region and Low-Quality Region with two qualities (both qualities have Pinch Points).

3.4. Minimal cross-plant transfer schemes

The headers targeting for single quality/contaminant problem is straightforward, just using the Composite Curves as shown in Chin et al.

(2021b), with all the sources and sinks from all the plants stacked in the Site Source and Sink CC. The header lines can be easily drawn from the Site Source Composite Curves, with a mix of cross-plant sources. However, in the case of multiple qualities, the individual allocation of the



Fig. 12. Plant B send its unused sources (LQR) to Plant A (HQR higher than Site Pinch Points).



Fig. 13. Plant B send its unused sources (LQR) to Plant A (HQR). Plant A has a Higher Pinch Point than Site Pinch for Quality A but a Lower Pinch Point than Site Pinch for Quality B.



Fig. 14. Plant B cannot send its unused sources (LQR for Quality A, but HQR for Quality B) to Plant A (HQR) due to Pinch Point for Quality B for Plant B being higher than the Site Pinch.

Summary of possible cross-plant transfer schemes. Note that in this formulation, '>' means 'higher than/worst than', '<' means 'lower than/better than', '/' means 'or' and ' = ' means 'equals to.'

Supplier (From)	Receiver (To)	Conditions	Remarks				
HQR	LQR	Supplier > Site Pinch Receiver≤Site	Desirable, but supplier require sources from other plants≤Site Pinch				
		Supplier≥Site Pinch Receiver > Site	Unnecessary				
		Pinch Supplier < Site Pinch	Not desirable				
		Supplier = Site Pinch Receiver < Site Pinch	Possible, a supplier can only give up part of the HQR source				
		Supplier = Site Pinch Receiver = Site Pinch	Unnecessary				
LQR	HQR	Supplier > Site Pinch Receiver ≥<br Site Pinch	Not desirable				
		Supplier = Site Pinch Receiver	Desirable, so that receiver can give up the source for other plants				
		Supplier < Site Pinch Receiver≥Site Pinch	Ideal transfer. If receiver = Site Pinch can be used for other plants.				
		Supplier > Site Pinch Receiver≥Site Pinch	Not desirable				
HQR	HQR	Supplier = Site Pinch Receiver > Site Pinch	Possible if there are no other options, a supplier can only give up part of the HQR source. This should follow by LQR + HQR transfer				
LQR	LQR	Supplier > Site Pinch Receiver≤Site Pinch	It is possible if there are no other options, so that receiver can give up the source for other plants. This should follow by LQR + HQR transfer				



Fig. 15. Site-level headers mixed with cross-plant sources and sent to the demands/sinks.

headers (Fig. 15) should be checked when there are Pinch Points in various qualities. In this case, an iterative procedure is proposed to determine the headers' properties as well as the individual allocation as well-Fig. 16.

For site-level framework, the first step involves identifying the fresh resources and then cross-plant sources by analysing the Pinch Points of all plants through the Composite Curves. The flowrates of cross-plant sources are then to be minimised as well. With the minimal cross-plant sources, an iterative allocation procedure with the pre-set number of headers is determined first, with the freshwater requirement determined from an individual approach with a mathematical approach presented in Supplementary Materials- Appendix A. In the first iteration, the number of the header can be set to one (H = 1). It is then checked whether the number of the header is sufficient to fulfil the demands without incurring an increment on the fresh resource. If not, the number of headers is increased by one, and the procedure is repeated.

4. Case study

The data required for this study are presented in Table 2 for a single contaminant study and Table 3 for multiple contaminants problem. The data for a single contaminant study is from Fadzil et al. (2018), for which the contaminants are the Total Dissolved Solid (TDS). The multiple contaminants case study is an illustrative case consisting of contaminants A, B and C adapted from Chin et al. (2021b).

5. Results and discussion

5.1. Single quality

The procedure presented in Fig. 16 for site-level headers determination with minimal cross-plant transfers is utilised. The first two steps involve the Pinch Point identification and data extraction part. Table 4 shows the extracted plant data after the Pinch Points for each plant has been identified.

For data extraction, the sources which are presented in the HQR should not be used for other plants since they are used to fulfil the sinks. The unused sources in the LQR should be used to transfer to other plants instead of wasting them. Note that for Plant 1, SR5 is directly used to fulfil SK6. In this case, the Pinch Points for all the plants are: (Plant 1, Plant 2, Plant 3, Plant 4, Plant 5) = (150, 130, 350, 125, 130). By performing the single targeting for all the plants, the Pinch Point for the Total Site is 130 ppm (not shown). Plant 1 and Plant 3 (200 ppm and 350 ppm) have Pinches higher than the Site Pinch (130 ppm), and Plant 4 (125 ppm) has Pinch lower than the Site Pinch. In this case, in order to ensure the site-level Pinch Point is 130 ppm, Plant 1 and Plant 3 require other higher quality sources.

The Pinch Points for all plants and the site-level Pinch provides information on the cross-plant source transfer. Plant 1 and Plant 3 have Pinches which has higher contamination than the Site Pinch Point, while Plant 2 and 5 have Pinch Points equal to the Site Pinch Point. It can be seen that the Pinch-Causing source for Plant 4 has a concentration of 125 ppm (SR3), which is lower than Site Pinch Point (130 ppm). The SR3 allocated for the sinks in LQR can be replaced by a lower quality source (\geq 130 ppm) in HQR of other plants to preserve the 125 ppm source. However, all of the sinks for Plant 4 are actually in the HQR, and they are not removed. In this case, the LQR unused SR3 in Plant 4 can be transferred to other plants. The cross-plant transfer of (LQR to HQR only) should be enough to reach the overall fresh resource target.

Based on the explanation presented in Section 3.3 and Table 1, Plant 2, 4 and 5 can send their LQR unused sources, which are lower than or equal to Site Pinch Point to HQR of Plant 1 and Plant 3 (as both HQR are higher than Site Pinch). Plant 4 has LQR sources which have lower than the Site Pinch, and this source is more desirable. According to Chin et al. (2021b), it is better to transfer the 125 ppm source Across the Site Pinch with a larger difference, i.e. to Plant 3 with Pinch 350 ppm, instead of



Fig. 16. Site-level headers targeting and design for multiple qualities problems.

Table 2	
Total Site data	for a single contaminant case.

	Plant 1			Plant 2			Plant 3			Plant 4			Plant 5	
	F _{SR} (t/h)	C _{TDS} (ppm)		F _{SR} (t/h)	C _{TDS} (ppm)		F _{SR} (t/h)	C _{TDS} (ppm)		F _{SR} (t/h)	C _{TDS} (ppm)		F _{SR} (t/h)	C _{TDS} (ppm)
SR1	200	50	SR1	50	50	SR1	100	130	SR1	20	50	SR1	20	130
SR2	80	100	SR2	250	100	SR2	120	290	SR2	80	100	SR2	100	130
SR3	80	100	SR3	150	130	SR3	85	300	SR3	100	125	SR3	40	250
SR4	140	150	SR4	150	250	SR4	200	350	SR4	100	150	SR4	25	400
SR5	200	200							SR5	50	800			
SR6	200	450												
					<u> </u>	—					<u> </u>			
	F_{SK} (t/h)	Z _{TDS} (ppm)												
SK1	200	0	SK1	50	20	SK1	100	0	SK1	20	0	SK1	20	0
SK2	80	50	SK2	250	50	SK2	120	100	SK2	80	25	SK2	100	50
SK3	80	50	SK3	150	100	SK3	85	125	SK3	100	25	SK3	40	80
SK4	140	100	SK4	150	200	SK4	200	300	SK4	100	50	SK4	25	100
SK5	200	120							SK5	50	100			
SK6	200	200												

Table	3
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Total Site data for multiple contaminants case.

	Plant 1					Plant 2					Plant 3			
	F _{SR} (t/h)	C _A (ppm)	C _B (ppm)	C _C (ppm)		F _{SR} (t/h)	C _A (ppm)	C _B (ppm)	C _C (ppm)		F _{SR} (t/h)	C _A (ppm)	C _B (ppm)	C _C (ppm)
SR1	45	15	400	35	SR1	45	15	400	35	SR1	15	140	105	15
SR2	34	117.7	12,500	168.2	SR2	34	150	250	169	SR2	15	205	55	40
SR3	8.01	103.8	45	125,000	SR3	59	110	45	125	SR3	10	410	205	55
SR4	19	22	120	30	SR4	19	22	120	30	SR4	11	5	10	5
SR5	44.8	225	229	307.5	SR5	43	225	229	305	SR5	25	600	230	35
SR6	170	4.7	1.2	2000	SR6	170	20	30	200	SR6	30	70	300	45
SR7	29	173.7	3500	205	SR7	29	150	350	205	SR7	20	250	1100	150
										SR8	25	150	660	90
_	F _{SK} (t/h)	Z _A (ppm)	Z _B (ppm)	Z _C (ppm)		F _{SK} (t/h)	Z _A (ppm)	Z _B (ppm)	Z _C (ppm)	_	F _{SK} (t/h)	Z _A (ppm)	Z _B (ppm)	Z _C (ppm)
SK1	45	0	0	0	SK1	45	0	0	0	SK1	15	5	7	5
SK2	34	17.6	294.3	33.1	SK2	34	8	94	33	SK2	15	5	7	5
SK3	8.01	3.7	20	5	SK3	59	3.7	20	5	SK3	10	25	100	15
SK4	19	0	0	0	SK4	19	0	0	0	SK4	11	30	130	20
SK5	815	7.5	200	17.5	SK5	890	7.5	160	17.5	SK5	25	200	210	50
SK6	170	0	0	0	SK6	170	0	0	0	SK6	30	150	100	20
SK7	29	3.7	20	5						SK7	20	475	300	100
										SK8	25	200	120	40

Plant 1 to reduce the number of the unnecessary transfer. The LQR unused sources from Plant 2 and Plant 5 (130 ppm) can be transferred to Plant 1 and Plant 3 as well. In return, Plant 2 or 5 requires sources from

other plants as well. In this case, the core cross-plant transfers that are feasible are.

Extracted plant data. '*' indicates Pinch Points, and red texts denote removed sources or sinks.

	Plant 1			Plant 2			Plant 3			Plant 4			Plant 5	
	F _{SR} /t/h	C/ppm		F _{SR} /t/h	C/ppm		F _{SR} /t/h	C/ppm		F _{SR} /t/h	C/ppm		F _{SR} /t/h	C/ppm
	HQR			HQR			HQR			HQR			HQR	
Fw	206.7	0		142.3	0		173.4	0		206	0		102.7	0
SR1	40	50	SR1	50	50	SR1	100	130	SR1	20	50	SR1	20	130
SR2	80	100	SR2	250	100	SR2	120	290	SR2	80	100	SR2*	62.3	130
SR3	80	100	SR3*	7.69	130	SR3	85	300	SR3*	44	125			
SR4*	133.3	150				SR4*	26.6	350						
	LOR Unused		LQR Unus	LQR Unused			LQR Unused			LQR Unused			LQR Unused	
SR4*	6.667	150	SR3*	79.8	130	SR4*	173.4	350	SR3*	56	125	SR2*	37.7	130
SR5*	0	200	SR4	62.5	250				SR4	100	150	SR3	40	250
SR6	200	450							SR5	50	800	SR4	25	400
	F _{SK} /t/h	Z/ppm		F _{SK} /t/h	Z/ppm		F _{SK} /t/h	Z/ppm		F _{SK} /t/h	Z/ppm		F _{SK} /t/h	Z/ppm
SK1	200	0	SK1	50	20	SK1	100	0	SK1	20	0	SK1	20	0
SK2	80	50	SK2	250	50	SK2	120	100	SK2	80	25	SK2	100	50
SK3	80	50	SK3	150	100	SK3	85	125	SK3	100	25	SK3	40	80
SK4	140	100	SK4	0	200	SK4	200	300	SK4	100	50	SK4	25	100
SK5	200	120							SK5	50	100			
SK6	0	200												

- (i) Plant 4 sends their sources (125 ppm) in LQR to Plant 3 HQR
- (ii) Plant 2 sends their sources (130 ppm) in LQR to Plant 1/3 HQR.
- (iii) Plant 5 sends their sources (130 ppm) in LQR to Plant 1/3 HQR.
- (iv) It is possible to send the LQR sources (350 ppm) from Plant 3 or (150 ppm) from Plant 1 to LQR of Plant 2 or 5 to replace the source with Site Pinch (130 ppm), but it is unnecessary since there are spare 130 ppm sources from Plants 2 and 5.
- (v) It is also possible for Plant 2 or 5 to give up the Site Pinch source (130 ppm) in the HQR for Plant 3, but this should be the last option since there are spare 130 ppm sources from both plants.

With these cross-plant transfer sources minimised, the total fresh resource target is identified as 822.2 t/h, which is still higher than the identified fresh resource target. Note that since new sources are available for each plant, the Pinch Points for individual plants can change as well. However, the changed Pinch Point usually is lowered for most of the cases, and new better quality sources can be transferred. This means the cross-plant transfer framework is iterative until the site-level fresh resource target is achieved.

The full explanation of the cross-plant transfer using the Pinch procedure for this case is not explained in detail, but the readers can refer to Chin et al. (2021b) for a detailed explanation of the cross-plant transfer frameworks. The readers could refer to Supplementary Materials- Appendix B. Table 5 below shows the results obtained between a fresh resource, cross-plant source transfer and a number of headers using the hierarchical framework proposed in Fig. 16. It is interesting to see that the least number of cross-plant headers is 3 in order to the required minimum fresh resources requirements.

5.2. Multiple qualities

For site-level headers synthesis, it is first required to determine the Pinch Points for all the three plants for the case study. Table 6 shows the plant data after the integration of individual plants are performed. The Composite Curves of individual plants are shown in Supplementary

Table 5

Number of headers set	Freshwater target/t/h	Cross-plant sources t/h	Cross-plant headers required
1	765.96	Infeasible	Infeasible
2	765.96	Infeasible	Infeasible
3	765.96	320.31	3
4	765.96	320.31	4

Material- Appendix C.

Based on the results, it can be shown that the Pinch Points for each plant are: Plant 1: {225 ppm, 12,500 ppm, 2000 ppm}, Plant 2: {110 ppm, ∞ , 200 ppm} and Plant 3: {600 ppm, 300 ppm, ∞ }. The total fresh resources required are about 2190 t/h. The minimum fresh resources and the Pinch Points for the Total Site can be identified using various methods such as Mathematical Programming, Pinch-based Composite Curves, Water Source Diagram and concentration potential. In this case, a mathematical approach is used for simplicity. It is identified that the fresh resources required are 2074.06 t/h, and the Pinch Points are {600 ppm, ∞ , 2000 ppm}. For a clearer demonstration of the site-level headers targeting procedure presented in Fig. 16, the study is divided into just two plants studies (Plant 1 and 2) and three plant studies (Plant 1, 2 and 3).

5.2.1. Two-plants (plant 1 and 2)

If the industrial site only contains two plants, the total minimal fresh resource is 2074.67 t/h, with Pinch Points {225 ppm, 12,500 ppm, 2000 ppm}, which follows the Pinch Points of Plant 1 for contaminants A, B and C. This means that Plant 1 is the limiting one, and its fresh resources can be further reduced. The current total fresh resource without site integration is 2079.6 t/h, which is higher than the fresh resource with site integration. It can be seen that the LOR of SR2 contains sources that have better qualities than the Site Pinches. Since the Pinch Points for Plant 2 are all lower than the Site Pinch Points, Plant 2 could send its LQR sources to Plant 1. The Pinch-Causing sources for Plant 2 are SR3 for contaminant A and SR6 for contaminants C. In fact, the LQR sources are all lower or equal to the Site Pinch Points, which all are feasible sources for Plant 1. Since Plant 1 is already at the Site Pinch Points, part of the Pinch-causing sources in Plant 1 can be replaced with Plant 2 LQR sources. By analysing the possible cross-plant transfer schemes in Table 1, the LQR sources from Plant 2 that can be transferred are:

(a) Plant 2 could send their sources in LQR (SR2-7) to Plant 1 HQR

By using the optimisation method, the SR6 from Plant 2 can be sent for Plant 1 as it requires minimal cross-plant flow transfer. The flowrate of the required cross-plant transfer is mainly to replace the SR2 in Plant 1. By using the optimisation method, it is determined that the flowrate of SR6 is 5.99 t/h. A single transfer from Plant 2 is enough to achieve the fresh resource for the Total Site (2074.7 t/h). Since only a single crossplant source, a single header is enough for both plants. Fig. 17 shows the header construction for two plants, where the SR6 from Plant 2 is the header source, and it is sent to SK2 and SK5 from Plant 1 (where the

Extracted plant data. '*' indicates Pinch Points, and red texts denote removed sources or sinks.

	Plant 1				Plant 2					Plant 3	Plant 3			
	F _{SR} (t/h)	C _A /ppm	C _B /ppm	C _C /ppm		F _{SR} (t/h)	C _A (ppm)	C _B (ppm)	C _C (ppm)		F _{SR} (t/h)	C _A (ppm)	C _B (ppm)	C _C (ppm)
	HQR					HQR					HQR			
Fw	1018.5				Fw	1061.1				Fw	47.36			
SR1	45	15	400	35	SR1	45	15	400	35	SR1	15	140	105	15
SR2	4.13	117.7	12,500*	168.2	SR3	47	110*	45	125	SR2	15	205	55	40
SR4	19	22	120	30	SR4	19	22	120	30	SR3	10	410	205	55
SR5	0.95	225*	229	307.5	SR6	45	20	30	200*	SR4	11	5	10	5
SR6	3.25	4.7	1.2	2000*						SR5	14.6	600*	230	35
SR7	29	173.7	3500	205						SR6	25.82	70	300*	45
	LQR Unus	ed			LQR U	Jnused				LQR U	Inused			
SR2	25.74	117.7	12,500*	168.2	SR2	34	150	250	169	SR5	10.42	600*	230	35
SR3	8.01	103.8	45	125,000	SR3	12	110*	45	125	SR6	4.18	70	300*	45
SR5	43.5	225*	229	307.5	SR5	43	225	229	305	SR7	20	250	1100	150
SR6	163.5	4.7	1.2	2000*	SR6	125	20	30	200*	SR8	25	150	660	90
					SR7	29	150	350	205					
	F _{SK} (t/h)	Z _A /ppm	Z _B /ppm	Z _C /ppm		F _{SK} (t/h)	Z _A /ppm	Z _B /ppm	Z _C /ppm		F _{SK} (t/h)	Z _A /ppm	Z _B /ppm	Z _C /ppm
SK1	45	0	0	0	SK1	45	0	0	0	SK1	15	5	7	5
SK2	34	17.6	294.3	33.1	SK2	34	8	94	33	SK2	15	5	7	5
SK3	8.01	3.7	20	5	SK3	59	3.7	20	5	SK3	10	25	100	15
SK4	19	0	0	0	SK4	19	0	0	0	SK4	11	30	130	20
SK5	815	7.5	200	17.5	SK5	890	7.5	160	17.5	SK5	25	200	210	50
SK6	170	0	0	0	SK6	170	0	0	0	SK6	30	150	100	20
SK7	29	3.7	20	5						SK7	20	475	300	100
										SK8	25	200	120	40



Fig. 17. Total Site headers allocation for multiple qualities: Two plants study.

results are from mathematical optimisation).

5.2.1.1. Three plants. For the three plants study, the Pinch Points for each plant are: Plant 1: {225 ppm, 12,500 ppm, 2000 ppm}, Plant 2: {110 ppm, ∞ , 200 ppm} and Plant 3: {600 ppm, 300 ppm, ∞ }. The total fresh resources required are about 2190 t/h. The fresh resources for the Total Site required are 2074.06 t/h, and the Pinch Points are {600 ppm, ∞ , 2000 ppm}. The Pinch Points for individual plants should be lower or equal to the Site Pinch Points. By analysing the Pinch Points and cross-plant schemes in Table 1, several insights can be identified:

- (i) Plant 1 can send its LQR sources as its Pinch Points for contaminants A & B are lower than the Site Pinch Points, and its Pinch Point for contaminant C is identical to Site Pinch. The receivers should have Pinches higher than the Site Pinches (Plant 3)
- (ii) Plant 2 can send its LQR sources as its Pinch Point for contaminants A, B & C are lower than the Site Pinch. The receivers should have Pinches higher than the Site Pinches (Plant 1 and 3)
- (iii) Plant 3 has Pinch Point for contaminant C higher than the Site Pinch, it can obtain sources transfer from other plants. It can send its LQR/HQR sources to other plants as well, provided receivers have Pinch Points lower than the Site Pinches.

For further fresh resource reduction, the Pinch Points for each plant

can be examined. The fresh resource for Plant 1 is limited by contaminant B as its Pinch Point is at 12,500 ppm, and it can be replaced by other sources. The candidate sources would be the LQR sources that have lower concentrations than the Pinch Points from Plant 2 and Plant 3. The ideal one would be SR3 and SR6 from Plant 2 since it has lower contaminants B, as discussed in the previous section. Plant 2 SR2 have lower qualities than SR3 in all contaminants, so SR3 should be used before SR2. The same reasoning applies to SR6 and SR5.

Plant 3 have potential LQR sources that are lower than the Site Pinch Points: SR7 and SR8. However, since SR8 has lower contaminants than SR7, SR8 should be prioritised. The Pinch-Causing sources from Plant 3 in the LQR region can be used as well (SR5 and SR6). Since Plant 3 has Pinch Point for contaminant C higher than the Site Pinch, it can obtain sources from other plants as well. The candidate source would be the Plant 1 SR6, which is the Pinch-causing source for contaminant C for Plant 1. The minimal total cross-plant transfers with detailed allocations are solved using mathematical optimisation. The minimal cross-transfer sources are determined as 108.9 t/h with minimal fresh resources. The procedure in Fig. 16 is then used to determine the number of headers required. By solving the number of headers iteratively with the crossplant sources, it is determined that three headers are sufficient to cover the demands. Fig. 18 shows the header sources mix from each plant and its allocation to each sink. Table 7 shows the results obtained using the hierarchical framework from Fig. 16. However, it is interesting



Fig. 18. Total Site headers allocation for multiple qualities with min. cross-plant sources: Three plants study.

Table 7	
Results for multiple qualities problem with headers.	

Number of headers set	Freshwater target/t/h	Cross-plant sources t/h	Cross-plant headers required
1	2074.67	Infeasible	Infeasible
2	2074.67	Infeasible	Infeasible
3	2074.67	108.9	3
4	2074.67	108.9	4

Results for multiple qualities problem with headers.

Constraints set	Freshwater target/t/h	Cross-plant sources/t/h	Cross-plant headers required
Min. number of transfers	2074.67	112.96	3
Min. cross-plant sources	2074.67	108.9	3

to see that if a minimum number of transfers is set, the total cross-plant sources is 112.96 t/h, which is slightly higher than 108.9 t/h (minimum cross-plant sources flow) – see Table 8. This is due to the fact that a minimum number of transfer reduce the mixing options of the sources, causing more sources required, but can reduce the number of piping connection. Higher cross-plant sources require more pumping power, which may require higher cost as well.

6. Conclusion

This work has proposed a header targeting and design approach for Total Site Water Integration problems using the Material Recovery Pinch Diagram for strategising minimal cross-plant transfer. The fresh resource targets for individual plants are identified, and the site-level target is first to be identified using various approaches. The main idea of the cross-plant transfer is to ensure the Pinch Points for individual plants are lower or equal to the Site Pinch Points while ensuring the cross-plant transfer is minimal without violating the minimal fresh resource usage. This work also provides a concept of determining the Pinch Points in the multiple qualities case. Several cross-plant transfer schemes are proposed to minimise the transfer of the cross-plant sources for single or multiple qualities cases, as shown:

- (i) When the source supplier/sender has Pinch(s) higher than the Site Pinch(s), the supplier can give up part of their HQR sources to LQR of receivers which have lower than or equal to the Site Pinch (s). The purpose is to use the high-quality sources from the receiver, and the supplier HQR would require sources from other plants with lower than or equal to Site Pinch(s)
- (ii) When the source supplier has Pinch(s) equal to the Site Pinch(s), they can give up part of their HQR source for receiver LQR lower than Site Pinch(s). Another possibility would be for the supplier to send the LQR sources to receiver HQR (lower or higher than Site Pinch). This is to preserve the high-quality source from the receiver as well.
- (iii) The ideal scenario would be the supplier LQR is lower than the Site Pinch(s), and they can send the sources to receiver HQR, which are higher or equal to Site Pinch(s). This guarantees reduction of fresh resources for the overall system.
- (iv) Transfer within regions (HQR to HQR or LQR to LQR) is possible but provided the transfer involves/across the Site Pinch Points and no other options available. The transfer also should be followed by a transfer LQR to HQR to guarantee overall fresh resource or waste reduction.

A header targeting framework is proposed using either a Pinch-Based approach or using mathematical approaches. The cross-plant transfer problem can be formulated as a problem to minimise the number of transfers (number of connections) or minimise cross-plant sources (pumping power). From case study 2, different objectives can yield different cross-plant sources flowrates, i.e. 112.96 t/h when the objective is to minimise cross-plant sources flow and 108.90 t/h when the objective is set to minimise the number of cross-plant connections.

For the multiple contaminants case, the individual source-to-sink allocation defines the Pinch Points and specify the vertical shifting of the Sink/Source CC (where sinks' contaminant limits are not reached Below the Pinch). It is an iterative procedure to check whether the header mix is feasible with the source-to-sink allocation for multiple contaminants cases. In this work, the source-to-sink allocation strategy is to fulfil all the contaminant limits (where the sources are conflicting) for every sink as much as possible. Different approaches can be used to determine the individual source-to-sink allocation first, and then the Composite Curves can be drawn to determine the Pinch Points. After Pinch Points are identified, the minimum cross-plant transfer schemes can be identified accordingly.

The concept proposed in this study can be useful for practitioners to determine a strategy of minimal cross-plant transfer while ensuring minimum resources requirements. With the insights from the Composite Curves, they can help to strategically plan for the various material recycling networks involving transfers between stakeholders. The solutions obtained can be combined with mathematical approaches and reduce the computation loads. For future method development, specific distances and geographical locations of the headers can be considered, coupled with the analysis as shown in this work. Different subsidy and tax policies can be studied to facilitate an economic-balanced eco-industrial park with maximum resources recycling rate. The concerns of the cost and footprint for the eco-industrial park planning should be addressed as well.

Author contributions

Hon Huin Chin: Conceptualisation, Methodology, Writing - original draft; Jiří Jaromír Klemeš: Supervision, Funding acquisition, Project management, Writing - review & editing; Sharifah Rafidah Wan-Alwi: Method Validation, Writing - review & editing;

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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