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Concentration potential concepts: Powerful tools for design of water-using networks with multiple contaminants

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ABSTRACT

This paper reviews concentration potential concepts and their applications in the design of water-using networks (WUNs) with multiple contaminants. The concentration potential concepts were proposed to determine the concentration order of water streams of multiple contaminants based on the overall allocating possibility of source streams to demand streams on the analogy of single contaminant WUNs. The precedence order of water-using processes, which is crucial for the network design, can be effectively identified by the values of Concentration Potential of Demands (CPDs). The concentration potential concepts, which were originally presented for the water networks of fixed contaminant load model, up to now have been successfully used to design a verity of water-using networks. Computing software has also been developed by combining the concentration potential concepts and linear programming approach. The methods proposed based on the concentration potential concepts have the advantages of simple calculation and clear engineering meaning. The results obtained based on the concentration potential concepts are comparable to that obtained by the literature methods. It is shown that the concentration potential concepts are powerful tools for the design of WUNs with multiple contaminants.
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1. Introduction

Water scarcity and water pollution have severely constrained the sustainable development of world economy and society. As an efficient technique for saving freshwater and reducing sewage, water network integration has been attracting more and more attention in process system engineering (PSE) field (Klemeš, 2012).

Water-using operations can be modelled as either fixed contaminant load (FL) or fixed flowrate (FF) ones (Prakash and Shenoy, 2005). The FL operations are implemented by mass-transfer units (e.g., scrubber, washing tower and extraction tower) which aim at removing a given amount of contaminant mass loads. The mass load of contaminant k removed (M_k) is shown in Eq. (1):

$$M_k = F_i\left(C_{i,k}^{\lim,out} - C_{i,k}^{\lim,in}\right) \quad (1)$$

where F_i is the flowrate of water-using process i, $C_{i,k}^{\lim,in}$ and $C_{i,k}^{\lim,out}$ are the limiting inlet concentration and limiting outlet concentration of contaminant k in process i. The FF operations do not involve mass transfer (e.g., boiler, cooling tower and reactor). For an FF operation, the inlet and outlet flowrates are specified and do not have to be equal. In addition, the outlet concentrations must reach their limiting values (Teles et al., 2009).

Pinch Analysis Methods and mathematical programming approaches are two prevailing techniques for the WUN integration (Klemeš et al., 2013). Wang and Smith (1994) introduced Water Pinch Analysis method, which stemmed from heat exchange network integration, into wastewater minimization for FL-model WUNs. Shortly after, a variety of pinch-based methods were developed by other research groups. The representative methods of them are as follows. Dhole et al. (1996) presented Source and Sink Composites (concentration vs. flowrate diagram) for targeting FF systems. Hallale (2002) put forward Water Surplus Diagram method to fill in the gap of

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Dhole et al. (1996) that pinch point was not unique. El-Halwagi et al. (2003) provided a rigorous graphical approach for targeting resource conservation networks. They identified Material Recycle/Reuse Pinch Point by developing a contaminant load vs. flowrate Source/Sink Composite Curve. Manan et al. (2004) established a numerical alternative to the Water Surplus Diagram of Hallale (2002), Water Cascade Analysis (WCA) technique, to yield accurate water targets by eliminating iterative steps. The WCA technique was suitable for targeting both FL and FF operations and multiple types of water-using operations. Prakash and Shenoy (2005) also developed a contaminant load vs. flowrate Composite Curve, which was independent of the work of El-Halwagi et al. (2003), and presented the nearest neighbours algorithm for designing FL and/or FF networks. Gomes et al. (2007) proposed Water Source Diagram technique to synthesise mass-exchange WUNs for different cases such as reuse, regeneration reuse, and water loss. Foo (2009) reviewed in detail the state-of-the-art Pinch Analysis Methods developed until 2008, especially those developed for the FF water-using systems. Shenoy (2011) gave rise to a Unified Targeting Algorithm (UTA) for the targeting of various resource conservation networks. The UTA table can be correspondingly converted into a Limiting Composite Curve or Grand Composite Curve for visualisation purpose. Deng et al. (2011) proposed a process-based graphical approach (PGA) by improving the Limiting Water Profile. With the PGA, the targets and design of a total water network involving both FL and FF operations can be obtained simultaneously. More recent state-of-the-art and detailed descriptions were presented in a handbook edited by Klemeš (2013). Parand et al. (2014) developed an Extended Composite Table Algorithm to target total water networks with a specified post-regeneration concentration and then proposed a Composite Matrix Algorithm to find the feasible region and the maximum value for post-regeneration concentration.

The pinch-based methods mentioned above have the advantages of simple calculation and clear engineering insight, but they are usually used to deal with single contaminant networks. When solving batch water networks, specific approaches such as Time Slice Composite Curves and Time Average Composite Curves have to be used.

The mathematical programming methods are the widely used approaches for the integration of WUNs with multiple contaminants. Analogical to heat integration, mathematical programming methods for WUN integration generally includes three steps (Klemeš and Kravanja, 2013): constructing a superstructure including all possible interconnections, formulating mathematical models, and developing solving strategies for the models. Mathematical programming method was initially used to optimise the water allocation network by Takama et al. (1980), but it did not receive attention until Doyle and Smith (1997) presented a solving procedure, in which initial values for nonlinear programming (NLP) were provided with a linear model (LP). Later, many other solving strategies were developed: recursive decomposition-based procedure involving mixed integer linear programming (MILP) relaxations (Alva-Argaez et al., 1998), branch-and-bound search (Koppol et al., 2004), heuristic strategy for good initial point to solve NLP (Chang and Li, 2005), spatial branch-and-contract procedure with MILP-based piecewise-affine relaxation (Karuppiah and Grossmann, 2006), giving initial values by LP relaxation of bilinear terms (Faria and Bagajewicz, 2010), global optimisation involving logic cuts using BARON software (Khor et al., 2012), and so on. Khor et al. (2014) gave a review of representative researches centring on mathematical programming methods for synthesis of single-site and continuous water networks. Several methods were developed recently to address the complex synthesis problem of multiple contaminant WUNs. Halim et al. (2015) applied a genetic algorithm (GA) based non-domination methodology to the multi-objective optimisation of total water networks. With the GA approach, very large-scale complex problems can be solved without resorting to heuristics or reduction optimisation strategies. Poplewski (2015) presented a new model to optimise the reuse/recycle water networks with data uncertainties and developed a multi-step solving strategy according to the theorem of corner points. Rubio-Castro et al. (2016) established a superstructure for optimising agriculture water networks and formulated it as an MINLP problem to obtain the economic, environmental and social benefits simultaneously. There has been also a potential to apply P-graphs to solve this problem (Lam, 2013).

By using mathematical programming approaches, the calculation in designing multiple contaminant WUNs can be fast. However, it is usually very complex to formulate an accurate superstructure and solve the models established. Moreover, the solving process is, unlike Process Integration, a “black box” operation, which causes the solutions are deficient in clear engineering insight.

In a conventional way, the water-using processes are connected directly by pipes. For a plant with many processes, the water network would become very complicated. Minor variations of flowrate or concentrations of upstream processes might affect the operation and control of downstream processes. To meet the traditional engineering objective of “keep it simple (Polley and Heggs, 1999)”, Feng and Seider (2001) proposed the concept of internal water mains for a water network. An internal water main can be considered as a reservoir (or tank) with a uniform contaminant concentration(s). Compared to a conventional network, the freshwater consumption of the network with internal water mains will increased at some level. Therefore, there is a trade-off between the saving in freshwater consumption and the number of water mains. Wang et al. (2003) developed a method for the design of multiple contaminant WUNs with one internal water main based on a concept of water-saving factor proposed. Zheng et al. (2006) presented a general method to design the WUNs with multiple internal water mains. Ma et al. (2007) put forward a design method for the WUNs with one or multiple water mains by combining a few heuristic rules with mathematical programming approach.

It can be seen from the above discussion that mathematical programming approaches are the main tools for the synthesis of WUNs with multiple contaminants. However, this kind of approach is of heavy computational burden and deficient in clear engineering insights. To address this problem, Liu et al. (2009) proposed methodology concepts of concentration potential. The concepts are presented based on the overall allocating possibility of source streams to demand streams on the analogy of single contaminant WUNs. With the concepts, the concentration order of the water streams of multiple contaminants can be identified and the design procedure of WUNs can be simplified considerably. In most cases, the results obtained with the concentration potential methods are comparable to those obtained with literature methods. This paper gives a review of concentration potential concepts and their applications in the design of WUNs.

2. Concentration potential concepts

The targeting and design of a WUN with multiple contaminants is more difficult than that of a WUN with single contaminant. For a WUN with single contaminant, the freshwater target and network design can usually be obtained without complication by two stages (Liu et al., 2004): (1) rank the processes in the order of limiting inlet concentration and perform the processes according to this order; (2) determine the stream allocation by mass balance. Table 1 shows the limiting data of a single contaminant WUN taken from Wang and Smith (1994). The inlet stream of a process (P) is designated as demand (D) and outlet stream as source (S) (Dhole et al., 1996). Correspondingly, $C^{\lim,in}$ is the limiting concentration of demand and

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