

# Design of Property-based Water-using Networks with the Operator Potential Concept and a Linear Programming Approach

Lei Zhang<sup>a</sup>, Ai-Hong Li<sup>b</sup>, Zhi-Yong Liu<sup>a,\*</sup>

<sup>a</sup>School of Chemical Engineering, Hebei University of Technology, Tianjin 300130, China

<sup>b</sup>Department of Chemical Engineering, Chengde Petroleum College, Hebei 067000, China  
 liuzhiyong@hebut.edu.cn

A new method is proposed in this article to design the property-based water-using networks with reuse. The operator potential concept and a linear programming approach are combined in the design procedure. The precedence order of demands is determined by the values of the operator potential of demands. The allocations of the sources to the demands are decided with a linear programming approach. The results of two literature examples obtained with the proposed method are comparable to that obtained with graphical or mathematical programming method in the literature. In addition, the proposed method can be applied to both single and multiple property systems.

## 1. Introduction

With the growing shortage of water resources and the increasingly strict regulations for water pollution, water system integration, one of the most effective techniques to save freshwater and reduce wastewater discharge, has become a research focus in chemical engineering field. Research on the integration of concentration-based water-using networks has nearly become mature (Fan et al., 2018). However, concentration is not the only constraint that limits the reuse and discharge of water streams in industrial processes. Other properties, such as pH, toxicity and density, also play important role in the allocation of water streams. Property integration (El-Halwagi et al. 2004) has received extensive attention.

For properties, some mixing rules (e.g., composition and chemical oxygen demand) are linear, but others (e.g., density and Reid vapor pressure) are nonlinear. To avoid numerical complications with these nonlinearities, Shelly and El-Halwagi (2000) proposed a concept called “clusters” to track the properties of streams. The concept of clusters was further defined as property operator, and the mixing rule of the property operator is linear (Kazantzi and El-Halwagi, 2005). To simplify the calculation in the design of property-based water networks, property operators are often used. Ponce-Ortega et al. (2010) summarized the property operators used in the literature.

Direct reuse is one of the primary measures for reducing freshwater consumption and wastewater discharge. Wen et al. (2013) presented a ternary diagram method to design water networks. An available region approach was proposed to facilitate the source-sink matching and determine the flowrate target. Deng et al. (2014) presented an improved ternary diagram approach for the synthesis of property-based resource conservation networks with direct reuse/recycling. Aiming at the design of the property-based water-allocation and heat-exchange networks, Zhou and Li (2015) proposed a strict and novel mathematical programming model based on state-space framework. Yang et al. (2015) developed a multi-property water-integrated superstructure model by considering environmental constraints. Deng et al. (2018) proposed a superstructure-based method for the design of property-based water networks. The mathematical model established in their work includes correlation equations for property operators, flowrates and mass balance constraints, and property constraints between different water plants. Gou et al. (2019) established a superstructure-based method for the design of property-based water networks including semi-continuous operation with the consideration of environmental constraints.

It can be seen from the above discussions that there are graphical approaches and mathematical programming methods for the design of property-based water networks. Graphical approaches can only solve the problems with less than three properties. Mathematical programming methods can deal with complex water networks, but the calculation load is often very heavy. In this paper, the operator potential concept (Zhang and Liu, 2011) and a linear programming (LP) approach are combined to design the property-based water-using networks. The values of operator potentials of demands (OPDs) will be used to identify the precedence order. An LP approach will be used to determine the allocations of sources to demands. With this method, the calculation load can be greatly reduced. Two literature examples are investigated to show the design procedure proposed.

## 2. Problem statement

The problem addressed in this article can be stated as follows: given are (a) a set of demand streams with known flowrates and limits on the property levels; (b) a set of source streams with known flowrates and properties; (c) a set of fresh sources with different purities, which can be used to satisfy the demand streams. The objective is to design property-based water-using networks with the minimum freshwater usage.

## 3. The new method

### 3.1 Operator potential concept

Liu et al. (2009) pointed out that it is important to determine the concentration order of water streams in the design of multi-contaminant water-using networks. They presented the concept of concentration potential of demand (CPD) to determine the concentration order of demand streams. Similarly, Zhang and Liu (2011) proposed the concept of operator potential of demand (OPD) for the design of property-based water-using networks.

The value of operator potential of demand (OPD) reflects the overall possibility of a demand to reuse the sources. The definition of OPD is shown in Eq(1):

$$OPD = \sum_{i=1}^{NS} R_{i,j} \quad (1)$$

where NS is the number of source streams,  $R_{i,j}$  is the allocation ratio of source streams to demands, which can be obtained with Eq(2):

$$R_{i,j} = \min_{k=1} \left[ R_{i,j}^k \right] \quad (2)$$

where  $R_{i,j}^k$  is the quasi-allocation ratio when each single property operator is considered and it can be calculated by Eq(3):

$$R_{i,j}^k = \min \left[ \frac{\psi_{Dj,k}^U - \psi_{Dj,k}^L}{\psi_{Si,k}^U - \psi_{Dj,k}^L}, \frac{\psi_{Dj,k}^U - \psi_{Dj,k}^L}{\psi_{Dj,k}^U - \psi_{Si,k}^L} \right] \quad (3)$$

where  $\psi_{Dj,k}^U$  is the upper bound of property operator for property k of demand j,  $\psi_{Dj,k}^L$  is the lower bound, and  $\psi_{Si,k}$  is the property operator for property k of source i.

The lower the value of OPD for a demand, the lower the overall possibility for the demand to reuse the sources. Therefore, the demand with the smallest OPD value should be satisfied first in the design procedure.

### 3.2 Design procedure

Similar to the work of Liu et al. (2009), a new design procedure is presented for the property-based water-using networks involving reuse as follows:

1. Arrange the demands in the ascending order of their OPD values.
2. Satisfy the demand with the lowest OPD value first. The demands are satisfied by internal source streams and freshwater:

$$F_{Dj} = \sum_{i=1} (F_{Si,j} + F_{fr,j}) \quad (4)$$

where  $F_{D_j}$  is the flowrate for demand  $j$ ,  $F_{S_{i,j}}$  is the segregated flowrate for source stream  $i$  allocated to demand  $j$ ,  $F_{fr,j}$  is the flowrate of freshwater allocated to demand  $j$ .

3. An LP approach is used to determine the allocations of sources to demands. The objective function of LP is as follows:

$$\min J = F_{fr} \quad (5)$$

The objective function shown in Eq(5) is subject to the following constraint:

$$F_{D_j} \times \Psi_{D_{j,k}}^L \leq \sum_j (\Psi_{S_{i,k}} \times F_{S_{i,j}}) + \Psi_{fr,j,k} \times F_{fr,j} \leq F_{D_j} \times \Psi_{D_{j,k}}^U \quad (6)$$

4. Return to step 2 until all the demands are satisfied.

## 4. Case studies

### 4.1 Example 1

This example is taken from Saw et al. (2011) and the limiting data are shown in Table 1. This is a single-property process with 2 demand streams and 2 source streams. One freshwater source shown in Table 1 is available. The values of OPD can be obtained with Eq(1), as shown in Table 2.

Table 1: Limiting data for Example 1

Demands	Flowrate	Operator, max	Sources	Flowrate	Operator, max
$D_j$	(kg/s)	$\Psi$ (atm <sup>1.44</sup> )	$S_i$	(kg/s)	$\Psi$ (atm <sup>1.44</sup> )
D <sub>1</sub>	5.0	4.87	S <sub>1</sub>	4.0	13.20
D <sub>2</sub>	2.0	7.36	S <sub>2</sub>	3.0	3.74
			Fresh	-	2.713

Table 2: Operator potentials of Example 1

Demands	D <sub>1</sub>	D <sub>2</sub>
OPD	1.67	2.53
Order	1	2

According to the OPD values shown in Table 2, D<sub>1</sub> should be satisfied first. The allocations of sources to D<sub>1</sub> are determined by an LP approach. The objective function is the minimum consumption of freshwater.

For satisfying D<sub>1</sub>, let the flowrate of S<sub>1</sub> be  $x$  kg/s, the flowrate of S<sub>2</sub> be  $y$  kg/s and the flowrate of freshwater be  $z$  kg/s. Then we have:

$$\begin{cases} x + y + z = F_{D_1} \\ x\Psi_{S_1} + y\Psi_{S_2} + z\Psi_{fresh} \leq F_{D_1} \times \Psi_D^U \\ \min J = z \end{cases} \quad (7)$$

The optimal solution can be obtained with MATLAB software as:  $x=0.7346$  kg/s,  $y=3$  kg/s,  $z=1.2654$  kg/s. Similarly, D<sub>2</sub> can be satisfied next. The final property operators are shown in Table 3.

Table 3: The property operators and flowrates of the demands of Example 1

Demands	Flowrate (kg/s)	Operator (atm <sup>1.44</sup> )
D <sub>1</sub>	5	4.87
D <sub>2</sub>	2	7.36

The final design is shown in Figure 1. From Figure 1, it can be seen that the freshwater consumption is 2.3792 kg/s and the interconnection number is 6. All the above results are the same as that obtained by Saw et al. (2011) with graphical method.

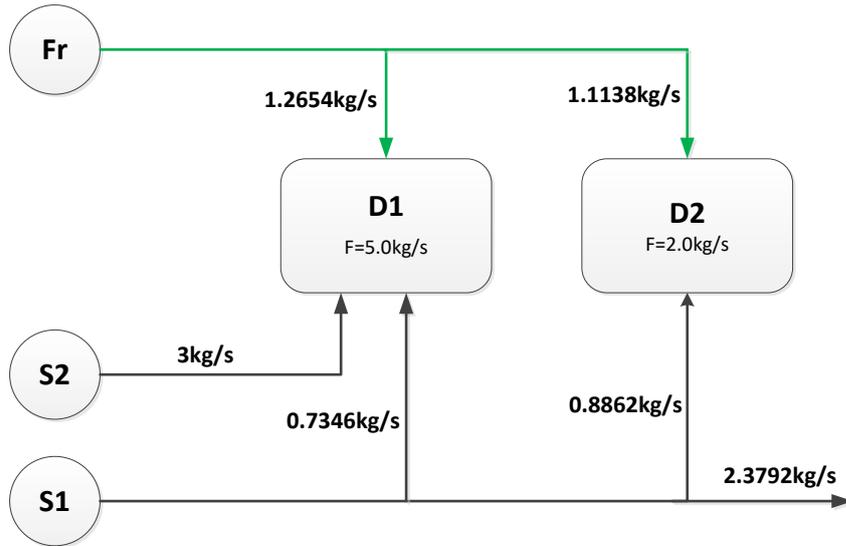


Figure 1: The final design for Example 1

#### 4.2 Example 2

The example is taken from Kheireddine et al. (2011), with the limiting data of sources and demands shown in Tables 4 and 5. Two freshwater sources are available, one with high purity and the other slightly contaminated. The OPD values calculated with Eq(1) are listed in Table 6.

Table 4: Limiting data of source streams and freshwater for Example 2

Sources	Flowrate (kg/h)	Impurity, $z_i$	Temperature (°C)	Vapour pressure (kPa)	pH
Washer101	3,661	0.016	75	38	5.4
Decanter101	1,766	0.024	65	25	5.1
Washer102	1,485	0.220	40	7	4.8
Freshwater1		0.000	25	3	7
Freshwater2		0.012	35	6	6.8

Table 5: Limiting data of demand streams for Example 2

Demands	Flowrate (kg/h)	Impurity		Temperature (°C)		Vapour pressure (kPa)		pH	
		Max	Min	Max	Min	Max	Min	Max	
Wash101	2,718	0.013	60	80	20	47	4.5	7	
Wash102	1,993	0.013	30	75	4	38	4	8	
Neutralizer	1,127	0.1	25	65	3	25	4.5	7	

Table 6: Operator potentials of Example 2

Demands	Wash101	Wash102	Neutralizer
OPD	1.40	1.41	1.99
Order	1	2	3

Table 7: The properties for demands of Example 2

Demands	Flowrate (kg/h)	Property			
		$Z_{\text{phenol}}$ (ppm)	Temperature (°C)	Vapour pressure (kPa)	pH
Wash101	2,718	0.013	65.63	33.03	6
Wash102	1,993	0.013	63.39	31.54	6
Neutralizer	1,127	0.1	49.59	19.01	5

The properties reaching their maximum are shadowed in the table

According to the OPD values shown in Table 6, Wash101 should be satisfied first. Wash102 and Neutralizer will be satisfied in turn. The final properties of demands are shown in Table 7, in which the properties reach their maximum value are shadowed. From Table 7, it can be seen that at least one property reaches the maximum value for all demands. The final design is shown in Figure 2.

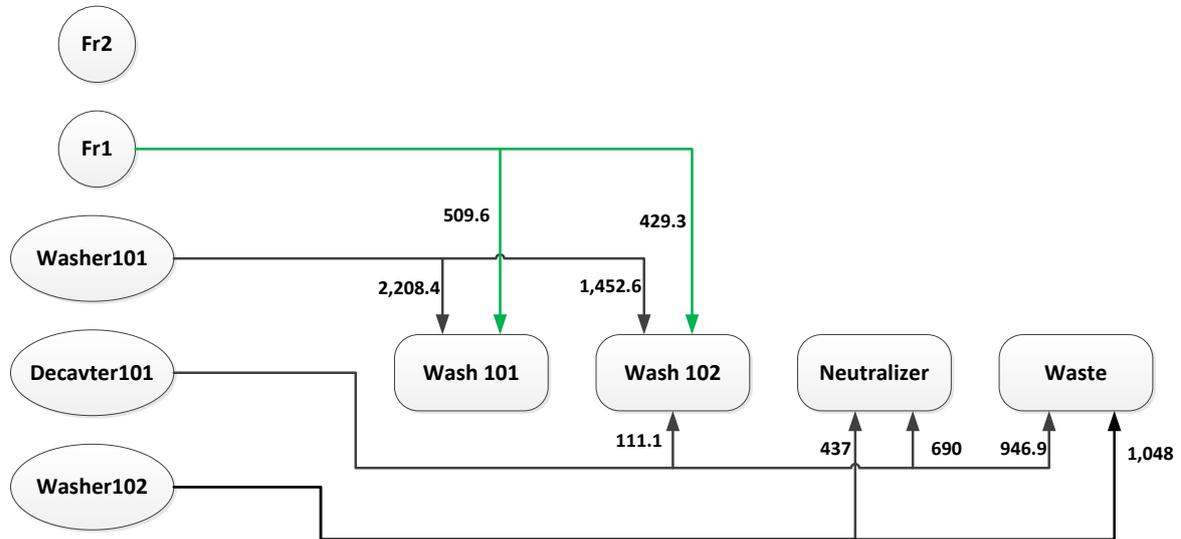


Figure 2: The final design for Example 2

Table 8: Comparison of the results for Example 2

	Freshwater (kg/h)	Wastewater (kg/h)	Interconnection number
This work	938.9	2,012.9	9
Kheireddine et al. (2011)	1,175.46	2,767.6	11

From the data shown in Table 8, it can be seen that the design obtained in this work is better than that obtained with mathematical programming method (Kheireddine et al., 2011). The above two examples show that the calculation of the proposed method is simple.

## 5. Conclusions

In this paper, a new method for the design of property-based water-using networks is proposed by combining the operator potential concept with a linear programming approach. The operator potential values are used to determine the precedence order of demands. The allocations of sources to demands are identified by using an LP approach. The proposed method can be applied to the water networks with single or multiple properties. The investigation for two literature examples shows that the method proposed can be used to solve the problem of property integration effectively. In addition, the calculation procedure of the proposed method is simple. However, the limitations of the proposed approach are as follows: firstly, the local optimal solutions might be obtained due to the usage of LP method in the allocations of sources to demands; secondly, the environmental restrictions of wastewater are not considered in the design. We will solve the problems in our future work.

## Acknowledgments

This work is supported by the Natural Science Foundation of Hebei Province, Hebei, China (Grant No. B2017202073) and the Science Research Foundation of Hebei Education Department, China (Grant No. ZD2019028).

## References

- Deng C., Jiang W., Zhou W., Feng X., 2018, New superstructure-based optimization of property-based industrial water system, *Journal of Cleaner Production*, 189, 878-886.
- Deng C., Wen Z., Foo D.C.Y., 2014, Improved ternary diagram approach for the synthesis of a resource conservation network with multiple properties. 1. Direct reuse/recycle, *Industrial & Engineering Chemistry Research*, 53, 17654-17670.
- El-Halwagi M.M., Glasgow I.M., Qin X., Eden M.R., 2004, Property integration: Componentless design techniques and visualization tools, *AIChE Journal*, 50, 1854-1869.
- Fan X.Y., Li A.H., Klemeš J.J., Liu Z.Y., 2018, Advances in designing and targeting of water systems involving regeneration/treatment units, *Journal of Cleaner Production*, 197, 1394-3407.
- Guo X.Z., Lin L.L., Zhang L., Du J., 2019, Property integration of batch process based on interceptors in semi-continuous operation, *CIESC Journal*, 70, 516-524.
- Kazantzi V., El-Halwagi M.M., 2005, *Chemical Engineering Progress*, 101, 28-37.
- Kheireddine H., Dadmohammadi Y., Deng C., Feng X., El-Halwagi M., 2011, Optimization of direct recycle networks with the simultaneous consideration of property, mass, and thermal effects, *Industrial & Engineering Chemistry Research*, 50, 3754-3762.
- Liu Z.Y., Yang Y., Wan L.Z., Wang X., Hou K.H., 2009, A Heuristic Design Procedure for Water-Using Networks with Multiple Contaminants, *AIChE Journal*, 55, 374-382.
- Ponce-Ortega J.M., El-Halwagi M.M., Jiménez-Gutiérrez A., 2010, Global optimization for the synthesis of property-based recycle and reuse networks including environmental constraints, *Computers & Chemical Engineering*, 34, 318-330.
- Saw S.Y., Lee L., Lim H.M., Foo D.C.Y., Chew I.M.L., Tan R.R., Klemeš J.J., 2011, An extended graphical targeting technique for direct reuse/recycle in concentration and property-based resource conservation networks, *Clean Technologies and Environmental Policy*, 13, 347-357.
- Shelley M.D., El-Halwagi M.M., 2000, Component-less design of recovery and allocation systems: a functionality-based clustering approach, *Computers & Chemical Engineering*, 24, 2081-2091.
- Wen Z., Deng C., Feng X., Zhu P., 2013, Ternary diagram approach for synthesis of property integration water network, *Journal of East China University of Science and Technology (Natural Science Edition)*, 39, 138-142.
- Yang C.L., Liu L.L., Du J., 2015, Water utilization networks integration with multiple-property based on environment and treated water reused, *CIESC Journal*, 66, 4916-4921.
- Zhang X.H., Liu Z.Y., 2011, A simple method for property integration, *Advanced Materials Research*, 6, 233-235.
- Zhou R.J., Li L.J., 2015, Simultaneous optimization of property-based water-allocation and heat-exchange networks with state-space superstructure, *Industrial & Engineering Chemistry Research*, 54, 9758-9769.