

Synthesis and Scheduling of Optimal Batch Water-recycle Networks*

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Abstract This work develops an optimization-based methodology for the design and scheduling of batch water recycle networks. This task requires the identification of network configuration, fresh-water usage, recycle assignments from sources to sinks, wastewater discharge, and a scheduling scheme. A new source-tank-sink representation is developed to allow for storage and dispatch tanks. The problem is solved in stages by first eliminating scheduling constraints and determining minimum usage of fresh water and wastewater discharge. An iterative procedure is formulated to minimize the total annual cost of the system by trading off capital *versus* operating costs. The work overcomes limitations in previous literature work including restricted recycle within the same cycle, lumped balances that may not lead to feasible solutions, and unrealistic objective functions. A case study is solved to illustrate the usefulness of the devised procedure.

Keywords process integration, process synthesis, mass integration, batch networks, water recycle, scheduling

1 INTRODUCTION

Water conservation is an important industrial objective. It contributes to the conservation of natural resources, reduction of negative environmental impact, and optimization of the cost of water usage and discharge. While much work has been undertaken in the area of designing water networks for steady-state applications (recent reviews including El-Halwagi [1], El-Halwagi *et al.* [2], Mann and Liu [3] and Bagajewicz [4]), much less work has been done on batch water processes. Given that batch systems are common within industry, it is important to develop batch water recycle networks that minimize fresh water consumption and wastewater discharge.

Wang and Smith [5] developed a time-pinch analysis method which uses graphical techniques to synthesize batch water networks. Majozi *et al.* [6] also devised a graphical technique which is an extension of the time-pinch analysis technique. In these works, water-using units are modeled as mass exchangers to deal with single-contaminant systems. Foo *et al.* [7] developed the water cascade analysis. In this method, mixing of water sources at different impurities in the same tank is not allowed. Kim and Smith [8] and Majozi [9, 10] developed mathematical formulations that optimize water usage and network configuration. These formulations are limited to mass transfer based water units and single contaminant systems. Chang and Li [11] also developed a mathematical formulation for batch networks that are not limited to mass transfer based water units. In spite of the usefulness of the previous research work, there is an opportunity for improvement to overcome the following limitations:

- (1) Recycle within the same cycle;
- (2) Lumped usage of water over a cycle;
- (3) Limited objective (*e.g.*, fresh-water minimization).

This article develops a systematic procedure to synthesize and schedule a cost effective batch water network. A source-tank-sink structural representation is developed to account for the potential configura-

tions of the water network. A hierarchical procedure is developed to solve the problem in interconnected stages and to establish tradeoffs between capital and operating costs.

This work also introduces novel ways to overcome all the aforementioned limitations. First, the limitation of same-cycle assignment is removed by permitting sources to be optimally recycled within the same batch cycle and/or storing and recycling sources to sinks in the following batch cycle. Second, the limitation of lumped usage of water over a cycle is avoided by implementing a two-tank arrangement when needed to allow for proper scheduling of recycled source water to sinks. Third, the objective function is extended to include the minimization of both the operating cost (fresh water) as well as the fixed cost of the network.

2 PROBLEM STATEMENT

The batch water network problem to be addressed in this work may be stated as follows.

(1) During a batch process with a given cycle time (τ), there are a number of water sources and sinks characterized by the following.

Sources There is a set $SOURCES = \{v | v = 1, 2, \dots, N_{SR}\}$ of process water streams. The dynamic profiles for the flow rate and composition of each source, v , are known and given by $w_v(t)$ and $y_{v,u}(t)$ where u is an index for components and t is the time from the beginning of the cycle ($0 \leq t \leq \tau$).

Sinks There is a set $SINKS = \{s | s = 1, 2, \dots, N_{SK}\}$ of process units that require water. Sinks can be a variety of units including washers, separators, reactors, *etc.* Constraints on dynamic profiles for the flow rate and maximum admissible composition of impurity of each sink s are known and given by $g_s(t)$ and $z_{s,u}^{max}(t)$.

(2) Available for service

A number of fresh water streams; each fresh stream r has given concentration of the u th impurity designated by $x_{r,u}$.

It is desired to develop a systematic procedure to

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synthesize and schedule a batch water network in which water from sources may be stored in tanks then recycled to sinks when needed or released as waste. The water network must be cost effective and meet all process constraints.

3 APPROACH

The following hierarchical procedure is proposed:

- (1) Targeting minimum usage of fresh water and minimum wastewater discharge;
- (2) Synthesis of a direct-recycle water network using storage and dispatch tanks to achieve the target;
- (3) Scheduling of an optimum operating scheme to achieve the target;
- (4) Tradeoff between fixed and operating costs.

The details of the proposed procedures are described in the following sections.

3.1 Multiperiod reformulation of sources and sinks

To avoid dealing with dynamic differential equations for sources and sinks, transformation to algebraic equations is undertaken *via* discretization. The discretization index is referred to as q . The q th time interval between indices $q-1$ and q is described by the following time interval $[t_{q-1}$ and $t_q]$. For the q th time interval, the quantity of the v th source is given by:

$$W_{v,q} = \int_{t_{q-1}}^{t_q} w_v(t) dt \quad (1)$$

and the composition of the u th component is given by

$$y_{v,q,u} = \frac{\int_{t_{q-1}}^{t_q} w_v(t) y_{v,u}(t) dt}{W_{v,q}} \quad (2)$$

To simplify the terminology, a single index, i , will be used for all discretized sources such that $i=1$ corresponds to $v=1$ and $q=1$, $i=2$ corresponds to $v=1$, $q=2$, and so on until $i=N_{\text{sources}}$ corresponds to $v=N_{\text{SR}}$ and $q=N_{\text{t_sources}}$. For each discretized source i , the flow and composition are referred to by W_i and $Y_{i,u}$. Similarly, for the constraints on the sinks:

$$G_{s,q} = \int_{t_{q-1}}^{t_q} g_s(t) dt \quad (3)$$

and the composition constraints are given by:

$$z_{s,q,u}^{\max} = \frac{\int_{t_{q-1}}^{t_q} g_s(t) z_{s,u}^{\max}(t) dt}{G_{s,q}} \quad (4)$$

Again, to simplify the index terminology, a single index, j , will be used for all discretized sink constraints such that $j=1$ corresponds to $s=1$ and $q=1$ until $j=N_{\text{sinks}}$ which corresponds to $s=N_{\text{SK}}$ and $q=N_{\text{t_sinks}}$. For each discretized sink j , the flow and composition constraints are referred to by G_j and $Z_{j,u}^{\max}$.

The structural representation involves the discretized sources and sinks as well as up to two sets of tanks: one for storage and one for dispatch. When the two sets are used, they alternate roles with storage in

one cycle and dispatch in the subsequent cycle. For the special case where only storage and dispatch tanks dominate the fixed cost of the network and fresh water and waste water treatment dominate the operating cost of the network, a hierarchical procedure is developed for this special case to solve the problem in interconnected stages. Benchmarks for minimum usage of fresh water and wastewater discharge are determined by eliminating scheduling constraints. An iterative procedure is formulated to minimize the total annual cost of the system by trading off capital *versus* operating costs.

3.2 Targeting for minimum fresh usage and wastewater discharge

The first step in the developed hierarchical procedure for the special case, where tanks dominate the fixed cost of the network, is to determine benchmarks for the operating cost of the network by identifying lower bounds for the usage of fresh water and the discharge of wastewater. One target is to determine the minimum flow of the fresh (which also corresponds to minimum discharge of the wastewater):

$$\text{Minimize } \sum_{r=1}^{N_{\text{fresh}}} \sum_{j=1}^{N_{\text{sinks}}} f_{r,j} \quad (5a)$$

where $f_{r,j}$ is the flow rate of the r th fresh assigned to the j th sink. Another objective is to determine the minimum cost of the fresh as follows:

$$\text{Minimize } \sum_{r=1}^{N_{\text{fresh}}} \sum_{j=1}^{N_{\text{sinks}}} C_r f_{r,j} \quad (5b)$$

Subject to
Splitting of sources

$$W_i = \sum_{j=1}^{N_{\text{sinks}}} w_{i,j} + w_{i,\text{waste}}, \quad i = 1, 2, \dots, N_{\text{sources}} \quad (6)$$

Waste flow

$$W = \sum_{i=1}^{N_{\text{sources}}} w_{i,\text{waste}} \quad (7)$$

Sink balances

$$G_j = \sum_{i=1}^{N_{\text{sources}}} w_{i,j} + \sum_{r=1}^{N_{\text{fresh}}} f_{r,j}, \quad j = 1, 2, \dots, N_{\text{sinks}} \quad (8)$$

$$G_j Z_{j,u} = \sum_{i=1}^{N_{\text{sources}}} w_{i,j} Y_{i,u} + \sum_{r=1}^{N_{\text{fresh}}} f_{r,j} x_{r,u}, \quad j = 1, 2, \dots, N_{\text{sinks}} \quad (9)$$

and $u = 1, 2, \dots, N_{\text{components}}$

Composition constraints for the sinks

$$Z_{j,u} \leq Z_{j,u}^{\max}, \quad j = 1, 2, \dots, N_{\text{sinks}} \text{ and } u = 1, 2, \dots, N_{\text{components}} \quad (10)$$

3.3 Minimizing fixed cost

The next step is to synthesize and schedule a

batch water network in which the fixed cost is minimized while still meeting the water targets determined in the previous step. The items which dominate the fixed cost are the storage and dispatch tanks. Therefore, the quantity of tanks is minimized using the following objective function:

$$\text{Minimize } \sum_{k=1}^{N_{\text{tanks}}} 2I_k \quad (11)$$

where I_k is a zero/one binary integer variable designating the absence/existence of a tank.

The following constraints are used:

Splitting of sources

$$W_i = \sum_{k=1}^{N_{\text{tanks}}} w_{i,k} + w_{i,\text{waste}}, \quad i=1,2,\dots,N_{\text{sources}} \quad (12)$$

Storage-tank balances

$$T_k = \sum_{i=1}^{N_{\text{sources}}} w_{i,k}, \quad k=1,2,\dots,N_{\text{tanks}} \quad (13)$$

$$T_k y_{k,u}^{\text{tank}} = \sum_{i=1}^{N_{\text{sources}}} w_{i,k} Y_{i,u}, \quad k=1,2,\dots,N_{\text{tanks}} \text{ and } u=1,2,\dots,N_{\text{components}} \quad (14)$$

$$T_k = \sum_{j=1}^{N_{\text{sinks}}} t_{k,j}, \quad k=1,2,\dots,N_{\text{tanks}} \quad (15)$$

Waste flow

$$W = \sum_{i=1}^{N_{\text{sources}}} w_{i,\text{waste}} \quad (16)$$

Sink balances

$$G_j = \sum_{k=1}^{N_{\text{tanks}}} t_{k,j} + \sum_{r=1}^{N_{\text{fresh}}} f_{r,j}, \quad j=1,2,\dots,N_{\text{sinks}} \quad (17)$$

$$G_j Z_{j,u} = \sum_{k=1}^{N_{\text{tanks}}} t_{k,j} y_{k,u}^{\text{tank}} + \sum_{r=1}^{N_{\text{fresh}}} f_{r,j} x_{r,u}, \quad j=1,2,\dots,N_{\text{sinks}} \text{ and } u=1,2,\dots,N_{\text{components}} \quad (18)$$

Composition constraints for the sinks

$$Z_{j,u} \leq Z_{j,u}^{\text{max}},$$

$$j=1,2,\dots,N_{\text{sinks}} \text{ and } u=1,2,\dots,N_{\text{components}} \quad (19)$$

Fresh flow

$$W_{\text{fresh}} = \sum_{r=1}^{N_{\text{fresh}}} \sum_{j=1}^{N_{\text{sinks}}} f_{r,j} \quad (20)$$

Furthermore, two more constraints are needed. First, assigning the integer values to used tanks: since the variable $I_k \in \{0,1\}$, it is necessary to add a constraint which assigns the value zero when there is no feed to the tank and one when there is feed to the tank. This can be accomplished by the following constraint:

$$T_k \leq U_k I_k, \quad k=1,2,\dots,N_{\text{tanks}} \quad (21)$$

where U_k is a given upper bound on the maximum capacity of the tank. When there is positive flow (T_k) to tank k , the variable I_k is forced to be one. On the

other hand, when T_k is zero, the constraint is satisfied by I_k being zero or one. However, the zero value will be picked in order to minimize the objective function.

Secondly, a constraint is added to include the value of the operating cost (either the minimum fresh cost target identified earlier or an iterative target for trading off fixed *versus* operating costs as will be described in the next section). Hence,

$$\sum_{r=1}^{N_{\text{fresh}}} \sum_{j=1}^{N_{\text{sinks}}} C_r f_{r,j} = \text{Cost} \quad (22)$$

3.4 Minimizing total annual cost

The last step in attaining a cost effective batch water network for the special case where tanks dominate the fixed cost of the network, is to achieve the minimal total annual cost (TAC) of the system by trading off fixed and operating costs. The proposed approach is shown by Fig. 1. First, the problem of minimizing the operating cost (minimizing fresh water consumption) is solved. The solution of this program provides the targets for fresh flow and wastewater discharge. Next, the fixed-cost minimization problem is solved subject to the identified fresh target. The solution identifies the assignment of sources to tanks and tanks to sinks, the associated flows, and the scheduling scheme. Inspection of the new design is done to try to further simplify the network. The solution is inspected to see if the two sets of tanks are needed for each assignment. If scheduling of any assignment can be done in one tank or without tanks, the unnecessary tanks are eliminated. Now that the network configuration has been determined, the TAC corresponding to this system can be calculated. Next, tradeoff of operating cost with fixed cost is done by decreasing the quantity of tanks used in the network by two. As seen in Fig.1, i is the subscript used for the tradeoff iterations. Therefore, $i-1$ is the iterative value calculated before iteration i . Then, the minimum operating cost (fresh water consumption) subject to the new tank constraint is determined. Further inspection of the new design is done to try to simplify the network. Comparison of the original minimum TAC and the new TAC (TAC i) is carried out. If the new annual cost is lower than the original, it will replace the original total annual cost as the current minimum. If not, the original TAC remains as the current minimum. Iterations are continued until a system of zero tanks is achieved (corresponding to the minimum fixed cost and maximum operating cost). The minimum stored value of the TAC is the most cost effective network and it provides sufficient information on the associated configuration and scheduling schemes.

4 CASE STUDY

Consider a batch process with the water sources and sinks. Tables 1 and 2 summarize the data for the sources and sinks. Available for use is one fresh water stream with a cost of \$0.20 per ton of water. Also, the cost of waste water treatment is \$0.30 per ton. Available

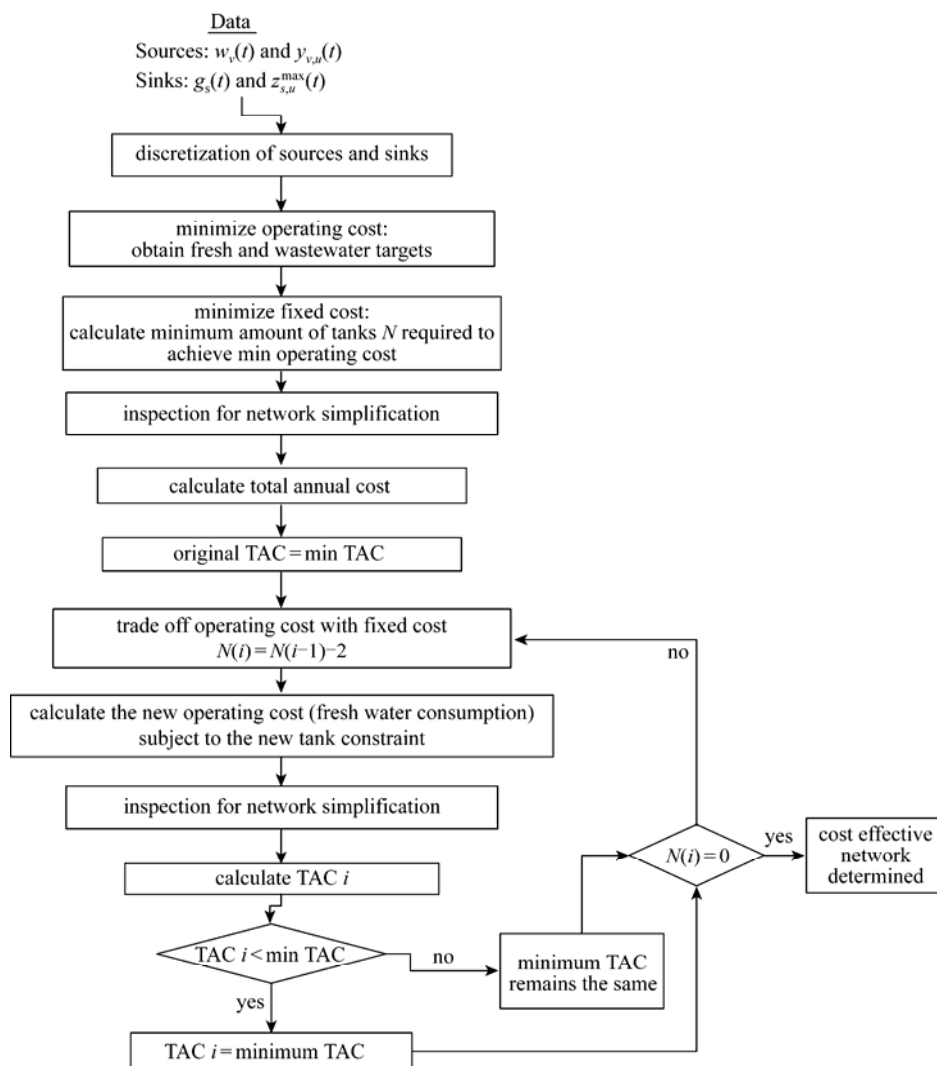


Figure 1 Minimum total annual cost approach

Table 1 Data for the process sources of the case study

Source number	Function for flow rate /t·h ⁻¹	Function for composition×10 ⁶ /kg·kg ⁻¹	Start time /h	End time /h
1	200.00	40($t+1$)	0	5
2	133.33	10($t-1$) ² + 20	1	4
3	[15.0($t-7$) + 70.0]×10	300	7	8

Note: t is time (h) from the start of the cycle.

are storage and dispatch tanks with an annual cost of \$35000 per tank and associated piping.

First, the dynamic profiles of sources and sinks are transformed into multi-period data by discretizing and integrating over eight equal intervals (1 h each). To determine the network with the minimum target for

fresh water usage and wastewater discharge, one must determine the minimum operating cost using the first mathematical formulation. The formulation is a linear program whose global solution provides 250 t of fresh water and 575 t of wastewater per batch cycle with an annual operating cost of \$243637 was found. Next, the hierarchical procedure was employed to trade off capital *versus* operating costs and to schedule and configure the network. Three iterations were performed with networks featuring four tanks, two tanks, and no tanks and the resulting total annual costs for these three configurations were found respectively to be \$383637, 377388, and \$545698. Therefore, the solution of \$377388 per year was selected. This network consists of 2 tanks, consumes 366.5 t of fresh water and generates 691.4 t of waste water per batch cycle.

Table 2 Data for the process sinks of the case study

Sink number	Flow rate demand /t·h ⁻¹	Constraint on lower bound on composition entering the sink×10 ⁶ /kg·kg ⁻¹	Constraint on upper bound on composition entering the sink×10 ⁶ /kg·kg ⁻¹	Start time /h	End time /h
1	290.00	0	80	1	6
2	100.00	0	350	3	7

Table 3 Legend for Fig. 3

Time/h	1a	1b	1c	2a	2b	3a	3b	4a	4b	5a
0-1	200 t	—	—	—	—	—	—	—	—	—
1-2	—	200 t	—	52.32 t	80.99 t	—	—	9.01 t	—	—
2-3	75.5 t	124.5 t	—	—	133.33 t	—	—	—	—	32.34 t
3-4	100 t	—	100 t	—	133.33 t	—	—	83.2 t	—	73.5 t
4-5	100 t	—	100 t	—	—	—	—	160 t	—	130.4 t
5-6	—	—	—	—	—	—	—	160 t	100 t	130.4 t
6-7	—	—	—	—	—	—	—	—	100 t	—
7-8	—	—	—	—	—	83.58 t	691.4 t	—	—	—

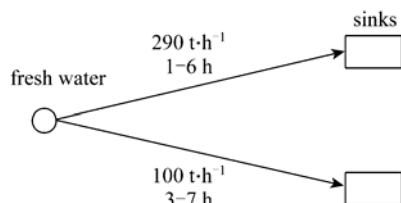


Figure 2 Original unintegrated network with a TAC of \$1119634

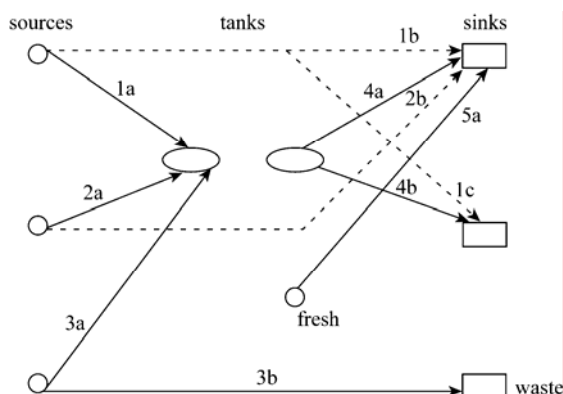


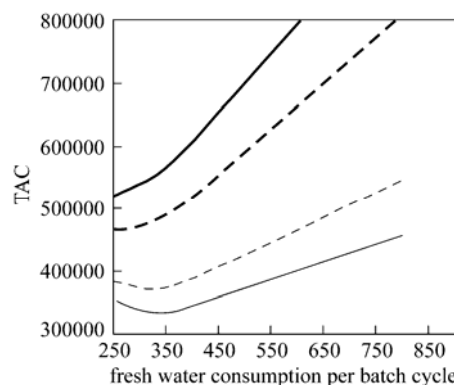
Figure 3 Optimized batch water recycle network with a TAC of \$377388

To further demonstrate the results of the optimized network, Figs. 2 and 3 illustrate the original unintegrated network and the optimized network respectively.

Comparing the annual cost of both networks, it is evident that it is economically beneficial to implement a batch water recycle network.

To further investigate optimization, sensitivity analysis is done on the price of fresh water. Fig. 4 illustrates the results.

As the cost of fresh water increases, both the operating cost as well as the TAC of the network increases. This increase has an effect on the optimization of the batch water recycle network. When the cost of fresh water is \$0.1 or \$0.2 per ton, it is determined that the optimal network is a network made up of two tanks and consumes 366.5 t of fresh water per batch cycle. As the cost of fresh water increases such as \$0.5 or \$0.7 per ton the optimal network is no longer a network of two tanks. Instead, the optimal design is a network of four tanks which consumes the minimum fresh water target of 250 t of fresh water per batch cycle.

Figure 4 Sensitivity analysis on fresh water cost
fresh water price: - - - \$0.2 per ton; - · - \$0.5 per ton;
— \$0.7 per ton; — \$1.0 per ton

5 CONCLUSIONS

This work has developed a novel systematic procedure to synthesize and schedule a cost effective batch water network. In addition to sources and sinks, two sets of tanks have been introduced for storage and dispatch. This new arrangement overcomes previous-research limitations that restricted assignment within the same batch cycle and were not capable of insuring sink feasibility when supply and demand overlap. The first step in the procedure determines water targets for both fresh water and wastewater by developing a representation with no scheduling limitations. This representation involves the use of infinite tanks which has been mathematically transformed into direct assignment of sources to sinks. Next, the problem of determining the minimum fixed cost or the minimum number of tanks has been formulated. Finally, an iterative procedure has been established to trade off operating and fixed costs (*e.g.*, by iteratively trading off fresh water consumption and number of tanks) until the minimum TAC is identified.

NOMENCLATURE

C_r	cost of fresh water stream r
$f_{r,j}$	flow of fresh water from stream r to discretized sink j
G_j	water demand of discretized sink j
I_k	zero/one binary integer variable designating absence/existence of tank k
N_q	number of multiple time periods per cycle

N_{sources}	number of discretized sources
N_{sinks}	number of discretized sinks
N_{SK}	number of process sinks
N_{SR}	number of process sources
T_k	water capacity of tank k
t	time, h
$t_{k,j}$	water flow from tank k to discretized sink j
U_k	upper bound on maximum capacity of tank k
W	total waste water
W_i	water flow of discretized source i
$w_{i,j}$	water flow from discretized source i to discretized sink j
$w_{i,k}$	water flow from discretized source i to tank k
$w_{i,\text{waste}}$	water flow from discretized source i to waste
$x_{r,u}$	composition of component u in fresh water stream r
$Y_{i,u}$	composition of component u in discretized source i
$y_{k,u}^{\text{tank}}$	composition of component u in tank k
$z_{j,u}$	composition of component u in discretized sink j
$z_{j,u}^{\text{max}}$	maximum admissible composition of component u to discretized sink j

Subscripts

I	discretized sources
j	discretized sinks
k	storage and dispatch tanks
q	discretization index for time intervals
r	fresh water stream
s	sinks
u	component
v	sources

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