

Report as of FY2006 for 2006TX229B: "Property-Based Management and Optimization of Water Usage and Discharge in Industrial Facilities"

Publications

Project 2006TX229B has resulted in no reported publications as of FY2006.

Report Follows

PROPERTY BASED MANAGEMENT AND OPTIMIZATION OF WATER USAGE AND DISCHARGE IN INDUSTRIAL FACILITIES

BY

ARWA RABIE

ABSTRACT

This work is aimed at developing a generally-applicable methodology for the optimal design of water recycle networks in batch processes. This is a challenging problem that requires the identification of network configuration, fresh-water usage, recycle assignments from sources to sinks, wastewater discharge, and a scheduling scheme. Previous research efforts have suffered from three primary limitations: restricted recycle within the same cycle, lumped balances that may not lead to feasible solutions, and unrealistic objective functions. These limitations are overcome by this work. A new source-tank-sink representation is developed to allow for storage and dispatch tanks. A hierarchical procedure is developed 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 annualized cost of the system by trading off capital versus operating costs. A case study is solved to illustrate the usefulness of the devised procedure.

INTRODUCTION, MOTIVATION, AND SIGNIFICANCE

Industries around the world are seeking efficient methods to conserve natural resources. Consequently, there is an ongoing drive towards increasing the utilization of process resources to decrease consumption of external resources. One of the most widely and extensively used resources in industry is water. In addition to its impact on natural resources and cost, excessive usage of water also leads to the discharge of significant quantities of wastewater. Consequently, responsible industries have begun to take considerable actions to identify ways to reduce fresh water consumption and wastewater generation. One effective approach has been to maximizing water reuse and recycle within the process plant. The numerous water sources and users must be simultaneously addressed. This leads to the need for efficient techniques to design water recycle networks to optimize the use of fresh water, recycle of process water, and discharge of wastewater.

Recently, significant contributions have been made in developing systematic techniques for the synthesis of industrial water networks. To date, the majority of the water-network research has

focused on continuous, steady-state processes. Recent reviews of steady-state water networks can be found in literature (e.g., El-Halwagi, 2006; El-Halwagi et al., 2003; Mann and Liu, 2000; Bagajewicz, 2000). Much less attention has been given to 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 (1995) developed a time-pinch analysis method which uses graphical techniques to synthesize batch water networks. This technique treats time as the primary constraint and concentration as the secondary constraint. Majozi et al. (2005) also devised a graphical technique which is an extension of the time-pinch analysis technique. Both of these techniques were limited to water-using units that are modeled as mass exchangers and deal with single-contaminant systems. Foo et al. (2005) devised a graphical method known as water cascade analysis which is limited to single contaminant systems. Also, mixing of water sources at different impurities in the same tank was not allowed. Kim and Smith (2004) and Majozi (2005a, b) 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 (2006) also developed a mathematical formulation for batch networks that are not limited to mass transfer based water units.

The previous research efforts have provided valuable tools and insights for batch water-network design. Nonetheless, they suffer from one or more of the following assumptions and limitations:

- Recycle within the same cycle: According to this assumption, water recycle is limited to units that require water later in the same cycle (i.e., no recycle from one batch cycle to another). In many cases, it may be beneficial to recycle water from a source which is available later in a cycle to a user which demands water earlier in the cycle. This can be achieved by storing water from one cycle and using it in another cycle.
- Lumped usage of water over a cycle: This assumption accounts for a total quantity and quality of water supply and demand. Such an assumption can lead to wrong results when the demand overlaps with the supply. As an illustration, consider the case shown by Fig. 1 with two water sources that are mixed and recycled to a water-demanding unit. Suppose that the first source is available from time t_1 to t_3 while the second source is available from time t_2 to t_5 . The quantities and compositions for sources I and II are given by W_I , W_{II} , y_I , and y_{II} , respectively.

The sink demands a total quantity of W_I+W_{II} of water. The maximum admissible composition to the sink is given by:

$$Z^{\max} = \frac{W_I y_I + W_{II} y_{II}}{W_I + W_{II}} \quad (1)$$

The two sources may be stored in a tank and used to provide feed to the sink. On a cycle basis, the stored mixture satisfies the sinks demand for water quantity and composition. However, there is a problem with implementation. When the sink begins to draw water at time t_4 , the composition of the stored mixture (of all source I and the quantity of source II generated from t_2 to t_4), will initially be satisfactory since it is less than Z^{\max} . However, as time progresses the concentration of the mixture will continually increase (since only higher-composition source II is contributing to the storage tank). Therefore, before reaching t_6 , the stored mixture will have a composition exceeding Z^{\max} . Since cycle-based averages do not capture such violation, this example underscores the need for detailed scheduling.

- **Fresh-water minimization:** The overwhelming majority of research on water-recycle networks has focused on the objective of minimizing fresh water usage and wastewater discharge. While this is a useful objective from an operating-cost perspective, it is also important to consider a more comprehensive objective dealing with the fixed cost in addition to the operating cost.

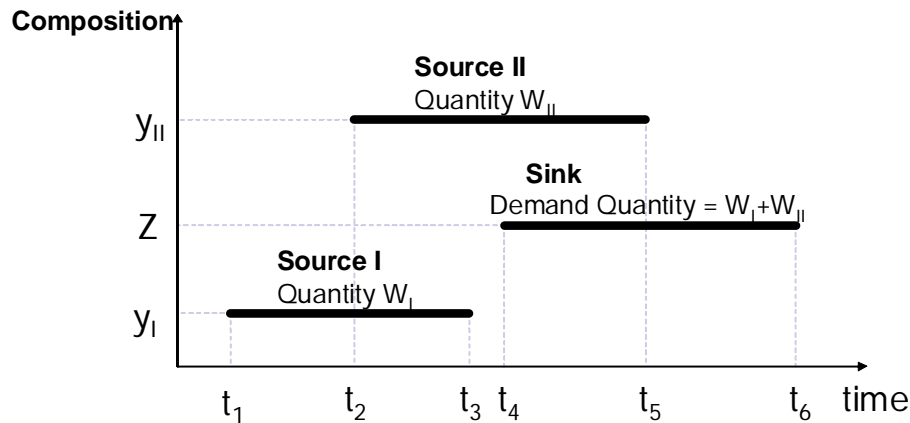


Fig. 1. Illustrating Example for Limitation of Averaging Supply

The objective of this paper is to develop a systematic procedure to synthesize and schedule an optimal batch water network of a minimum total annualized cost while meeting all process constraints. The aforementioned limitations of previous research efforts are overcome. A source-tank-sink structural representation is developed to account for the potential configurations of the water network. This representation allows for separate tanks to be used for storage and dispatch

over alternating cycles. A hierarchical procedure is developed to solve the problem in interconnected stages. First, the target for minimum fresh usage and waste discharge is identified. Next, a minimum fixed-cost network is synthesized using dispatch and storage tanks to meet the fresh and wastewater targets and to devise a scheduling scheme. Next, trade off occurs between capital and operating costs with the objective of minimizing total annualized cost. A case study is solved to illustrate the merits of the developed approach.

PROBLEM STATEMENT

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

During a batch process with a 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 flowrate 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. Constraints on dynamic profiles for the flowrate and maximum admissible composition of impurity of each sink s are known and given by $g_s(t)$ and $z_{s,u}^{max}(t)$.

Available for service are:

- A number of fresh water streams; each fresh stream r has an impurity concentration of x_r .

It is desired to develop a systematic procedure to 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 meet the minimum total annualized cost and meet all process constraints. The synthesis and scheduling tasks require the identification of the following:

- What is the optimum network configuration including assignment of sources and sinks?
- Which fresh stream(s) should be used? How much of each?
- How many tanks should be used? What are their sizes? What are their feeds?
- How should the synthesized network be scheduled for operation?

APPROACH

The following approach will be used to synthesize an optimal batch water network of minimum total annualized cost:

1. Reformulation of sources and sinks into discrete events
2. Target minimum usage of fresh water and minimum wastewater discharge
3. Synthesize a direct-recycle water network using storage and dispatch tanks to achieve the target
4. Schedule an optimum operating scheme to achieve the target
5. Tradeoff water usage, discharge, fixed and operating cost to obtain minimum total annualized cost

Due to the dynamic variation of both the sources and the sinks, the process sources and the sink constraints are discretized over time. Each source is discretized into a number of sources with a given composition and a given water quantity. The sink constraints are also discretized; each having a given water demand and a given maximum inlet impurity composition, i.e.

For the sources, the time domain is decomposed into $N_{t_Sources}$ time intervals (large enough to capture significant changes in composition). The discretization index is referred to as q . The q^{th} time interval between indices $q-1$ and q is described by t_{q-1} and t_q . The flowrate profile of each source, v , is transformed into a discrete set of flows per cycle (water quantities per cycle not continuous flowrates). For the q^{th} time interval, the quantity of the v^{th} source is given by:

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

and the composition is given by:

$$y_{v,q,u} = \frac{\int_{t_{q-1}}^{t_q} w_v(t) y_{v,u}(t) dt}{W_{v,q}} \quad (3)$$

To simplify the terminology, a single index, i , will be used for all discretized source such that $i=1$ corresponds to $v=1$ and $q = 1$. $i=2$ corresponds to $v=1$, $q=2$, $i=N_q + 1$ corresponds to $v=2$, $q=1$, and so on until $i= N_{Sources}$ corresponds to $v=N_{SR}$ and $q=N_{t_Sources}$. For each discretized source i , the flow and composition are referred to by W_i and $Y_{i,u}$.

Similarly, for the sinks, the time domain is decomposed into N_{t_Sinks} time intervals. An index p is used for discretization and the p^{th} time interval is described by t_{p-1} and t_p . The constraint for flowrate profile of each sink, s , is transformed into a discrete set of constraints on flows as follows:

$$G_{s,p} = \int_{t_{p-1}}^{t_p} g_s(t) dt \quad (4)$$

and the composition constraints are given by:

$$z_{s,p,u}^{max} = \frac{\int_{t_{p-1}}^{t_p} g_s(t) z_{s,u}^{max}(t) dt}{G_{s,p}} \quad (5)$$

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 $p = 1$ until $j= N_{Sinks}$ which corresponds to $s=N_{SK}$ and $p=N_{t_Sinks}$. For each discretized sink j , the flow and composition constraints are referred to by G_j and $Z_{j,u}^{max}$.

The foregoing discretization and reformulation are carried out as pre-synthesis tasks. Therefore, the problem formulation will involve algebraic equations instead of the simultaneous algebraic and differential equations.

STRUCTURAL REPRESENTATION

The next step in designing a batch water network is developing a structural representation which embeds all potential configurations of the network and enables proper scheduling. As mentioned before, earlier approaches have been restricted by two limitations: recycle within the same cycle and lumped usage of water over a cycle. These limitations can be overcome by the source-tank-sink representation shown in Fig. 2. According to this new representation, two sets of tanks are used: one set for storage and another for dispatch. Every cycle, the role of each set of tanks will alternate. During one cycle, the storage tanks will be collecting water from sources and in the next cycle, these tanks will be used to dispatch the stored water to the sinks. This arrangement shown by Fig. 2 allows the assignment of sources from one cycle to be allocated to sinks in the subsequent cycle. This is important in cases when a source available at time t_1 is to be assigned to a sink at time t_2 with $t_2 < t_1$. The storage-dispatch arrangement also insures proper

satisfaction of sink constraints even when source supply and sink demand overlap (as was shown by Fig. 1).

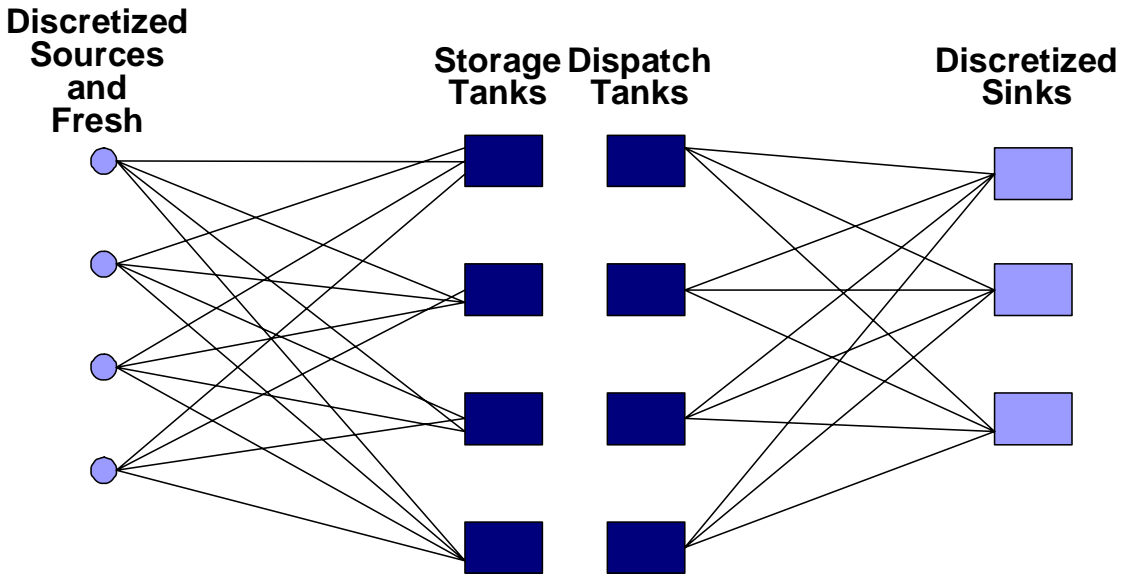


Fig. 2. Source-Sink Representation with Storage and Dispatch Tanks

Each source is split into several fractions that are allocated to storage tanks. The stored water are drawn from the dispatch tanks and assigned to sinks. One of the sinks is designated as the “waste sink” and it is intended to collect the unallocated sources.

TARGETING FOR MINIMUM FRESH USAGE AND WASTEWATER DISCHARGE

In order to determine benchmarks for the operating cost of the network, it is beneficial to identify lower bounds for the usage of fresh water and the discharge of wastewater. A particularly useful observation is that one of the key conditions for attaining minimum fresh usage is when there are no scheduling limitations for assigning any source to any sink. Eliminating scheduling limitations may be achieved by allowing the use of infinite number of storage and dispatch tanks. This arrangement allows all the sources to be available whenever any of the sinks demand them. Equivalently, the targeting problem can be dealt with by assigning sources directly to sinks. Therefore, the following mathematical formulation can be used to determine the water targets. One target is to determine the minimum flow of the fresh (which also corresponds to minimum discharge of the wastewater):

$$\text{Minimize } \sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{Sinks}} f_{r,j} \quad (6a)$$

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

$$\text{Minimize } \sum_{r=1}^{N_{Fresh}} \sum_{j=1}^{N_{Sinks}} C_r f_{r,j} \quad (6b)$$

Subject to

Splitting of sources:

$$W_i = \sum_{j=1}^{N_{Sinks}} w_{i,j} + w_{i,waste} \quad i=1, 2, \dots, N_{Sources} \quad (7)$$

Waste flow:

$$Waste = \sum_{i=1}^{N_{Sources}} w_{i,waste} \quad (8)$$

Sink balances:

$$G_j = \sum_{i=1}^{N_{Sources}} w_{i,j} + \sum_{r=1}^{N_{Fresh}} f_{r,j} \quad j=1, 2, \dots, N_{Sinks} \quad (9)$$

$$G_j Z_{j,u} = \sum_{i=1}^{N_{Sources}} w_{i,j} Y_{i,u} + \sum_{r=1}^{N_{Fresh}} f_{r,j} x_{r,u} \quad j=1, 2, \dots, N_{Sinks} \text{ and } u=1, 2, \dots, N_{Components} \quad (10)$$

Composition constraints for the Sinks:

$$Z_{j,u} \leq Z_{j,u}^{\max} \quad j=1, 2, \dots, N_{Sinks} \text{ and } u=1, 2, \dots, N_{Components} \quad (11)$$

The source-splitting constraints distribute the flows from the sources to the sinks and the waste. The waste flow is the sum of the unallocated sources. The sink balances account for the flow and component balances for the fresh water streams and the source streams.

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:

$$\text{Minimize } \sum_{k=1}^{N_{Tanks}} 2I_k \quad (12)$$

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:

$$W_i = \sum_{k=1}^{N_{Tanks}} w_{i,k} \quad i=1,2,\dots,N_{Sources} \quad (13)$$

Storage-tank balances:

$$T_k = \sum_{i=1}^{N_{Sources}} w_{i,k} \quad k=1,2,\dots,N_{Tanks} \quad (14)$$

$$T_k y_{k,u}^{Tank} = \sum_{i=1}^{N_{Sources}} w_{i,k} Y_{i,u} \quad k=1,2,\dots,N_{Tanks} \text{ and } u=1,2,\dots,N_{Components} \quad (15)$$

$$T_k = \sum_{j=1}^{N_{Sinks}} t_{k,j} + t_{k,waste} \quad k=1,2,\dots,N_{Tanks} \quad (16)$$

Waste flow:

$$Waste = \sum_{k=1}^{N_{Tanks}} t_{k,waste} \quad (17)$$

Sink balances:

$$G_j = \sum_{k=1}^{N_{Tanks}} t_{k,j} + \sum_{r=1}^{N_{Fresh}} f_{r,j} \quad j=1,2,\dots,N_{Sinks} \quad (18)$$

$$G_j Z_{j,u} = \sum_{k=1}^{N_{Tanks}} t_{k,j} y_{k,u}^{Tank} + \sum_{r=1}^{N_{Fresh}} f_{r,j} x_{r,u} \quad j=1,2,\dots,N_{Sinks} \text{ and } u=1,2,\dots,N_{Components} \quad (19)$$

Composition constraints for the Sinks:

$$Z_{j,u} \leq Z_{j,u}^{\max} \quad j=1,2,\dots,N_{Sinks} \text{ and } u=1,2,\dots,N_{Components} \quad (20)$$

Furthermore, two more sets of constraints are needed:

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.

Finally, 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,

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

MINIMIZING TOTAL ANNUALIZED COST (TAC)

The last step in attaining an optimal batch water network is to achieve the minimal TAC of the system by trading off fixed and operating costs. The proposed approach is shown by Fig. 3. 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, the second tank is 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. 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 TAC and the new TAC is carried out. If the new annualized cost is lower than the original, it will replace the original total annualized 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 global minimum TAC for the system and its associated configuration and scheduling are the optimum schemes.

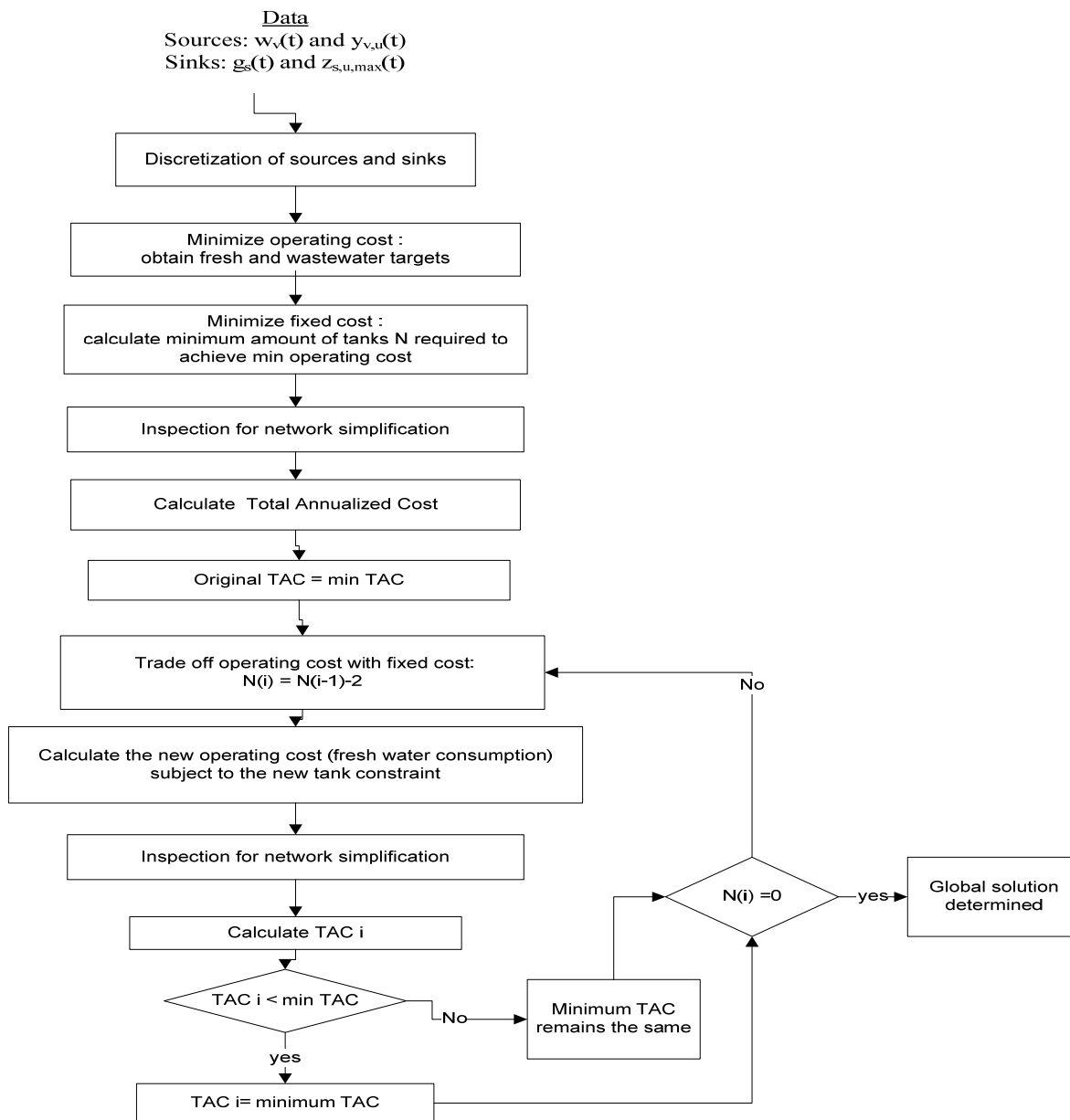


Fig. 3. Minimum TAC Approach

CASE STUDY

A batch water network in a manufacturing plant has a batch cycle of eight hours. It is a single contaminant system which consists of two water sources and two water sinks. Both the

sources and sinks exhibit dynamic behavior. Available for use is one fresh water stream with a cost of \$.21/kg of water. Also available are storage and dispatch tanks. The tanks cost \$1000/m³ and have an installation and yearly maintenance cost of \$1,000 and \$500 per tank respectively. The discretized source and sink data for this network is represented by the following tables.

Source Data:

Source	Hour	Y _i	W _i (kg)
1	1-2	0.00	0.0
	3-4	0.00	0.0
	5-6	0.05	20
	7-8	0.10	30
2	1-2	0.00	0.0
	3-4	0.85	30
	5-6	0.90	40
	7-8	0.00	0.0

Sink Data:

Sink	Hour	Z _{jmax}	G _j (kg)
1	2	0.50	50
	7	0.60	50
2	1	0.40	50
	8	0.70	50

Following the above procedure, the next step in synthesizing a batch water network is determining the minimum operating cost using the first mathematical formulation. The formulation is a linear program consisting of 22 constraints and 27 linear variables. A solution of 80 kg of fresh water and 0 kg of wastewater with a yearly operating cost of \$18,396 was found. Next, using the second mathematical formulation, the minimum fixed cost subject to the minimum operating cost must be determined. The formulation is a mixed integer non-linear program consisting of 41 constraints, 58 variables, 24 non-linear variables, and 4 integers. The solution of two tanks was

found with a total annualized cost of \$21,182. Using the iterative procedure presented above, \$21,182 is the minimum total annualized cost.

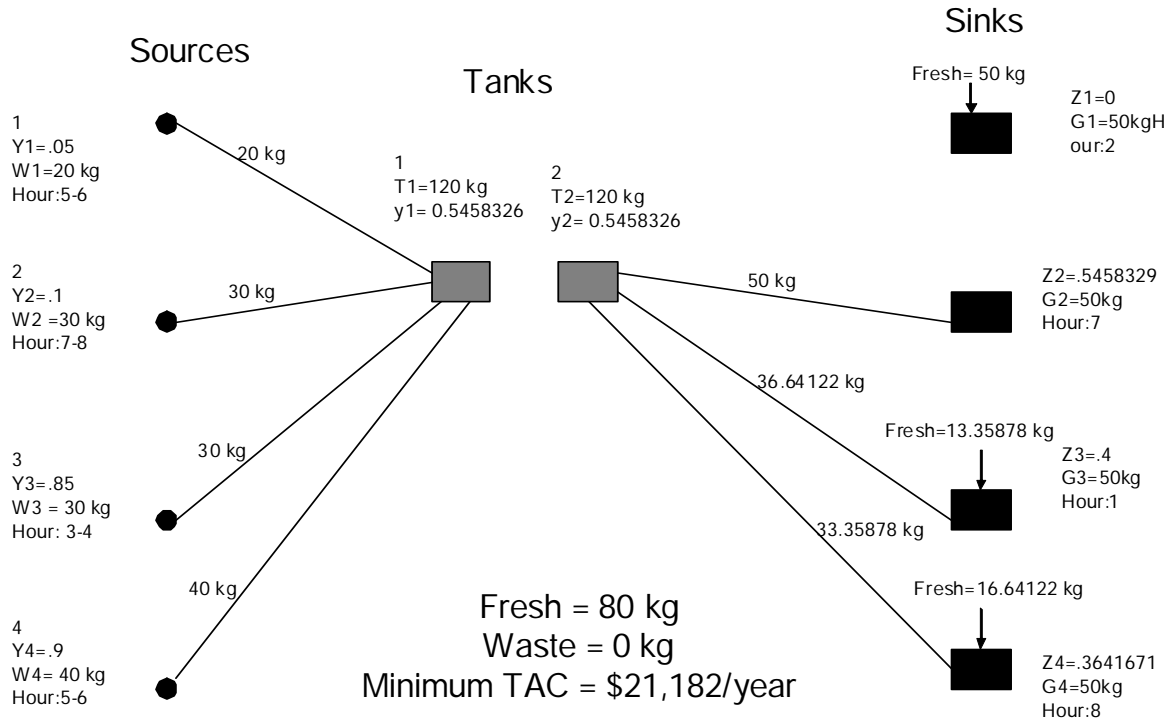


Fig. 4. Optimal Network for the Case Study

As illustrated above, two tanks are required to achieve the optimal batch water network. The storage tank will collect all the water from the four discretized sources. It will have an impurity composition of 0.5458, and will require a capacity of at least 120 kg. The dispatch tank will have the same impurity composition, and require the same capacity as the storage tank. It will begin by dispersing 36.64 kg of water to sink 3 at hour one of the cycle. Then it will disperse 50.00 kg of water to sink 2 at hour seven, and 33.36 kg of water to sink 4 at hour eight of the cycle. Sink 1 will acquire all of its water demand (50.00 kg) from the fresh source at hour two of the cycle. Overall, 80.00 kg of fresh water per cycle is required and no wastewater is generated.

CONCLUSIONS

This work has developed a novel systematic procedure to synthesize and schedule an optimum batch water network. First, a structural representation has been developed to embed

potential configurations. 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. Sources and sinks have been reformulated through discretization into meaningful events to transform simultaneous differential and algebraic equations into algebraic equations. Then, water targets for both fresh water and wastewater have been determined 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.

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- Will be presented in 2007 AIChE meeting

Property based management and optimization of water usage and discharge in industrial facilities

Arwa Rabie and Mahmoud El-Halwagi

Department of Chemical Engineering,
Texas A&M University

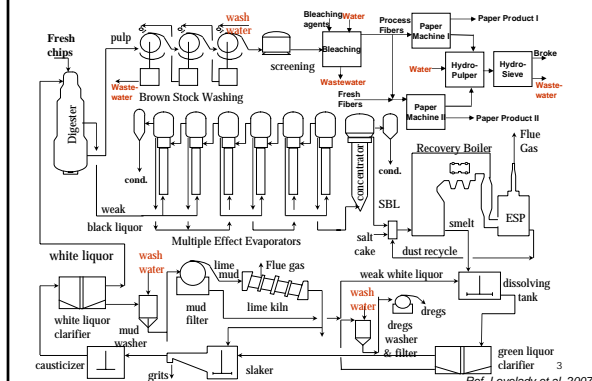
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Outline

- Motivation
- Problem Scope
- Literature Survey
- Problem Statement & Representation
- Novel Approach
- Case Study
- Conclusions

2

Motivating Example



3

Motivation

- Industrial facilities significantly use fresh water and discharge wastewater
- Growing public concern as well as environmental regulations
- Conservation of resources
- Enhanced market competitiveness

4

Problem Scope

Given: a batch process with a number of

- water sources whose composition and flow rate vary over time
- sinks whose water demand and maximum admissible composition vary over time

Objectives: Develop a systematic procedure to

- Synthesize an optimal batch water network
- Schedule an operating network of a minimum total annualized cost while meeting all process constraints

5

Examples of Previous Literature

- Wang and Smith(1995), Majozi (2005)
 - Graphical method limited to mass transfer based utilities
 - Limited to single contaminant systems
 - Used storage tanks
 - Water sources were not recycled to lower concentration utilities or in previous times of the cycle.
- Foo, Manan& Tan(2005)-Water Cascade Analysis
 - Graphical method for non-mass transfer based utilities
 - Limited to single contaminant systems
 - Water sources were not recycled to utilities that required water in previous times of the cycle.
 - Mixing of water sources at different impurities in the same tank was not allowed

6

Examples of Previous Literature

- Kim and Smith(2004), Majozi(2005a),Majozi(2005b)
 - Mathematical formulation limited to mass transfer based water units
 - Limited to single contaminant systems
 - Used storage tanks
 - Water sources were not recycled to utilities that required water in previous times of the cycle.
- Chang & Li(2006)
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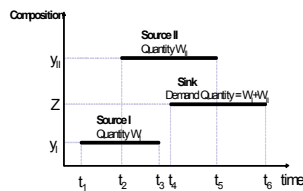
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Limitations of Previous Work

- One of more of the following limitations:
- Recycle within the same cycle: water recycle is limited to units that require water later in the same cycle
 - Lumped usage of water over a cycle: this assumption accounts for a total quantity and quality of water supply
 - The objective of minimizing fresh water usage: it is important to consider an objective dealing with fixed cost in addition of operating cost.
 - Lack of global solution procedure

8

Lumped usage of water



$$G_j = W_I + W_{II}$$

$$Z^{\max} = \frac{W_I Y_I + W_{II} Y_{II}}{W_I + W_{II}}$$

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Problem Statement

During a batch cycle (τ) of a given batch process there is a number of:

-Sources; process streams

- impurity concentration of $y_{i,j}(t)$
- flow of $w_i(t)$
- $0 \leq t \leq \tau$

-Sinks; process units that are in need of water

- maximum inlet impurity composition $z_{s,i}(t)$
- flow rate requirement $g_s(t)$
- $0 \leq t \leq \tau$

Available for service are:

-Tanks; used for water storage and dispatch

-Fresh water streams

- Impurity composition x_i
- cost of C_i

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Optimization Formulation

- Dynamic variation of sources and sinks
- Synthesis:
 - Numerous source and sink constraints
 - Tanks selection and assignment
- Scheduling:
 - When to store sources and when to dispatch them to sinks

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Mathematical programming approach

Characteristics and Features:

- Mathematical programs can tackle complex systems
- Need to handle multiple sources
- Need to handle multiple sink requirements
- Need to incorporate storage and dispatch tanks

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Novel Approach

- Reformulate sources and sinks into discrete events
- Determine target for minimum usage of fresh water and minimum waste water discharge
- Synthesize a direct-recycle water network using storage and dispatch tanks to achieve the water target
- Schedule an optimum operating scheme to achieve the target
- Use insight to further simplify network design
- Tradeoff water usage, discharge, fixed and operating costs to obtain minimum TAC

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Source Reformulation

During a batch cycle τ , the profile for both $w_v(t)$ and $y_{v,u}(t)$ are known ($0 \leq t \leq \tau$).

- $$W_i = \int_{t_{p-1}}^{t_p} w_v(t) dt$$
- $$Y_{i,u} = \frac{\int_{t_{p-1}}^{t_p} w_v(t) y_{v,u}(t) dt}{W_i}$$

Source water flow profile

Source composition profile

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Sink Reformulation

During a batch cycle τ , the profile for both $g_s(t)$ and $z_{s,u}(t)$ are known ($0 \leq t \leq \tau$).

- $$G_j = \int_{t_{p-1}}^{t_p} g_s(t) dt$$
- $$Z_{j,u}^{\max} = \frac{\int_{t_{p-1}}^{t_p} g_s(t) z_{s,u}^{\max}(t) dt}{G_j}$$

Inlet water requirement

Maximum Inlet Composition

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Water Recycle Network Representation

- Availability and demand are not concurrent.
- Assumption: two sets of tanks will be used one for storage and one for dispatch

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Targeting Mathematical Formulation

- Minimize $\sum_{j=1}^{N_{\text{Sinks}}} \sum_{i=1}^{N_{\text{Sources}}} C_i t_{i,j}$

Subject to:

- Splitting of Sources**

$$W_i = \sum_{j=1}^{N_{\text{Sinks}}} W_{i,j} + W_{i,\text{waste}} \quad i=1, 2, \dots, N_{\text{Sources}}$$
- Waste flow**

$$\text{Waste} = \sum_{i=1}^{N_{\text{Sources}}} W_{i,\text{waste}}$$
- Sink Balances**

$$G_j = \sum_{i=1}^{N_{\text{Sources}}} W_{i,j} + \sum_{u=1}^{N_{\text{Components}}} \ell_{j,u}$$

$$G_j Z_{j,u} = \sum_{i=1}^{N_{\text{Sources}}} W_{i,j} Y_{i,u} + \sum_{u=1}^{N_{\text{Components}}} \ell_{j,u} X_{j,u}$$

$$Z_{j,u} \leq Z_{j,u}^{\max} \quad j=1, 2, \dots, N_{\text{Sinks}} \text{ and } u=1, 2, \dots, N_{\text{Components}}$$

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Synthesis & Scheduling Mathematical Formulation

- Minimize $2 N_k$

Subject to:

- $$N_k = \sum_{i=1}^{N_{\text{Sources}}} I_i$$
- $$I_i \in \{0, 1\}$$
- $$T_i \leq U_i I_i$$
- Splitting of Sources**

$$W_i = \sum_{j=1}^{N_{\text{Sinks}}} W_{i,j} + W_{i,\text{waste}} \quad i=1, 2, \dots, N_{\text{Sources}}$$
- Storage Tank Balances**

$$T_k = \sum_{i=1}^{N_{\text{Sources}}} W_{i,k} \quad k=1, 2, \dots, N_{\text{Tanks}}$$

$$T_k Y_{k,u} = \sum_{i=1}^{N_{\text{Sources}}} W_{i,k} Y_{i,u}$$

$$T_k = \sum_{j=1}^{N_{\text{Sinks}}} t_{k,j} \quad k=1, 2, \dots, N_{\text{Tanks}} \text{ and } u=1, 2, \dots, N_{\text{Components}}$$

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Synthesis & Scheduling Formulation

Continued

- Waste Flow**

$$Waste = \sum_{i=1}^{N_{sources}} W_{i,waste}$$
- Sink Balances**

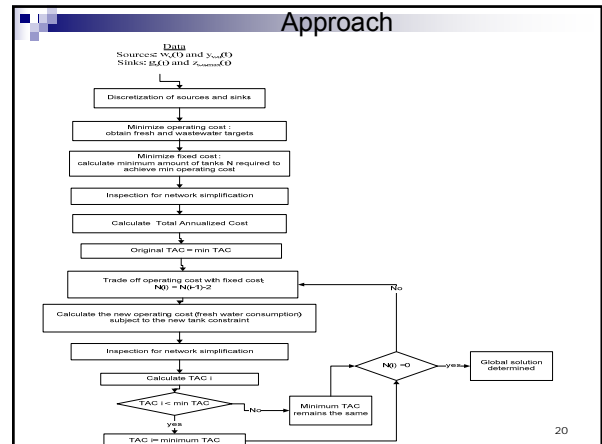
$$G_j = \sum_{i=1}^{N_{sources}} f_{i,j} + \sum_{i=1}^{N_{sinks}} f_{r,i} \quad j=1,2,\dots,N_{sinks}$$

$$G_j Z_{j,u} = \sum_{i=1}^{N_{sources}} f_{i,j} k_{i,u} + \sum_{i=1}^{N_{sinks}} f_{r,i} X_{r,u} \quad j=1,2,\dots,N_{sinks} \text{ and } u=1,2,\dots,N_{components}$$

$$Z_{j,u} \leq Z_{j,u}^{max} \quad j=1,2,\dots,N_{sinks} \text{ and } u=1,2,\dots,N_{components}$$
- Operating Cost Constraint**

$$\sum_{i=1}^{N_{sources}} \sum_{j=1}^{N_{sinks}} C_i f_{i,j} = Cost$$

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Case Study

Batch water network

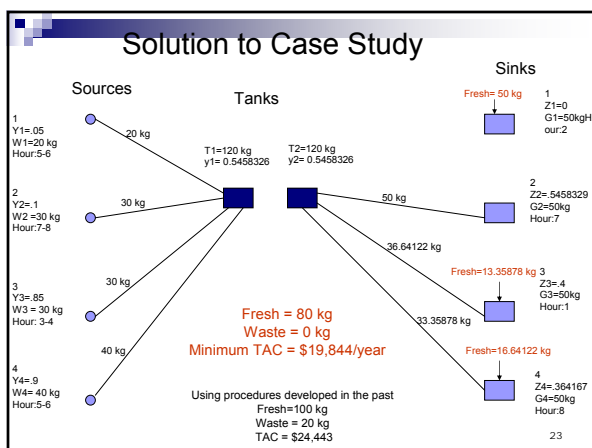
- 2 process sources
- 2 sinks
- 1 contaminant present in water from sources
- 1 fresh water stream
 $-x_i=0$
 $-cost: \$0.21/kg$
- Available tanks
 $-cost: \$1000/m^3$
 $-installation cost: \$1,000 \text{ per tank}$
 $-yearly maintenance: \$500 \text{ per tank}$
- Batch cycle = 8 hours

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Case Study

Source	Hour	Y _i	W _i (kg)
1	1-2	0.0	0
	3-4	0.0	0
	5-6	0.05	20
	7-8	0.10	30
2	1-2	0.0	0
	3-4	0.85	30
	5-6	0.90	40
	7-8	0.0	0
Sink	Hour	Z _{jmax}	G _j (kg)
1	2	.5	50
	7	.6	50
2	1	.4	50
	8	.7	50

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Conclusion

- Developed a systematic procedure to synthesize and schedule a batch water network
- Properly discretized batch cycle into meaningful events
- Targeting of water usage and discharge ahead of synthesis and scheduling
- Devised an iterative scheme to achieve total minimum annualized cost

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