AN EFFICIENT DECOMPOSITION ALGORITHM FOR A WEIGHED PROCESS

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Considering the computation load of process simulation, it is necessary to assign a weight to each stream of a chemical process. Therefore, tearing criteria for the weighed process are proposed, which minimize the number of cut streams (cycle intervals) first and then search for an alternative stream with the minimum weight for each detected cycle interval. Based on them, an efficient decomposition algorithm is then developed, with two parts. One is to detect the cycle interval, using the weighed reachable vector method. The other is to determine the cut stream for each cycle interval through three indispensable procedures (searching, judging and regulating). After searching out an alternative stream with minimum weight, judging is carried out by verifying whether the detected cycle interval is broken or not. Then regulating is implemented by modifying the local weighed adjacency matrix. These three procedures are repeated until the stream with minimum weight is got. Finally, the optimal cut-set is obtained.

Four test problems are examined. The proposed algorithm finds the minimum weighing sum for all these problems under the minimum number of cut streams.

Introduction

Currently the practical simulation systems are primarily based on the sequential modular approach[3], in which cyclic digraphs of process units are to be reduced into acyclic ones by tearing a set of selected streams. Then the cut streams become the interface between the system model and the iterative procedure for convergence. Each stream has a different influence on the computation load for iterative convergence according to its sensitivity, the number of variables and so on. Therefore, a set of cut streams (cut-set) should be selected under consideration of the computation load. Consequently, it is reasonable to assign a weight to each stream of a chemical process, and its weight reflects the degree of difficulty for convergence. In this paper, the decomposition (cut-set selection) algorithm is investigated, in which streams of the chemical process have already been weighed by some procedures.

Pho and Lapidus[8] studied the weighed process decomposition based on the concept of Signal Flow-Graph (SFG)[1], and proposed an algorithm termed the Basic Tearing Algorithm (BTA). Its algorithm uses a cumbersome approach of converting a digraph into a SFG; furthermore, the optimality of the solution cannot be guaranteed because both its algorithm and tearing criteria are insufficient. Later, Murthy and Husain[7] also studied the weighed process decomposition based on list processing[5], and developed the M & H-2 algorithm on the basis of the K & S algorithm[6], which is simple with hand calculation for a sizable flowsheet. Its algorithm is limited to weight assignment in which the weight of each stream is equal to the number of output streams of that node. Moreover, it is not suitable for decomposing a complex process.

For sequential modular process simulation, there are two factors which have a large effect on the computation load. One is the number of cut streams, which is generally correlated to the total number of iteration cycles. By decreasing one cut stream, one cycle iterative calculation can be reduced. The other is the weight of a cut stream, which is usually related to the computation load of that iteration cycle. The smaller the weight of the cut stream, the less the

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computation load in that cycle. Unfortunately, so far the widely used tearing criterion for the weighed process decomposition only minimizes the weighing sum of cut streams, which is not sufficient to decrease the computation load. Therefore, cut streams should be selected by considering both the two factors mentioned above. It is proposed as tearing criteria that the number of cut streams (counter stream intervals[9]) or cycle intervals) be minimized first and then for each detected cycle interval an alternative stream with minimum weight be searched. In this way the minimum weighing sum can be ensured under the condition of the minimum number of cut streams.

The purpose of this study is to develop an efficient decomposition algorithm for the weighed process based on the proposed tearing criteria. An efficient algorithm is developed under consideration of two points. One is to ensure the minimum number of cut streams. The other is to select the alternative stream with minimum weight after each cycle interval is detected. Thus the arithmetic weighing sum of the cut-set may be the minimum. In the proposed algorithm, the weighed reachable vector method is developed for the detection of cycle intervals (identification of counter streams), in which the weighed adjacency matrix is used instead of the adjacency one, so that an initial vertices sequence of a better order can be obtained. Moreover, three indispensable procedures (searching, judging and regulating) are developed for determining the cut stream with minimum weight for each detected cycle interval. When a cycle interval is detected, first an alternative stream with minimum weight is searched on the local weighed adjacency matrix. Then judging is carried out by verifying whether this stream breaks all the cycles in the detected cycle interval with the reachable vector operation or not. Finally, regulating is implemented by modifying the local weighed adjacency matrix according to the individual case. For each detected cycle interval, searching, judging and regulating are repeated. Because the cut stream with minimum weight is found out for each detected cycle interval, the optimal cut-set with minimum weighing sum can finally be obtained.

Four test problems collected by Husain[5]) are calculated. The effectiveness of the proposed algorithm is demonstrated through the solutions of these problems, in which not only the number of cut streams but also the weighing sum are minimum.

1. Tearing criteria

For the weighed process decomposition, the computation load, which is influenced largely by the number of cut streams and their weights, should be considered. Under the premise of reducing the cyclic digraphs into the acyclic ones, the following criteria are proposed.

1) minimize the number of cut streams.
2) minimize the weighing sum of cut streams under the condition of minimum number of cut streams.

In a detected cycle interval (a counter stream interval), it is known that an effective cut stream can break all cycles of this interval when it is cut. Therefore, it is possible to find out an alternative cut stream with minimum weight among the effective cut streams by the procedures of searching, judging and regulating. These procedures can be expressed in terms of the following equation.

$$W_i = \min\{w_j\} \qquad j = 1, 2, \cdots, l$$

where w_j and l are the weight of the j-th cut stream and the number of effective cut streams in the i-th cycle interval (counter stream interval[9])) respectively, and W_i is the minimum weight of these effective streams in the i-th cycle interval. Obviously the counter stream is an effective cut stream, so in any case there exists at least one effective cut stream in each detected cycle interval.

Searching, judging and regulating are repeated for all detected cycle intervals, so the weighing sum of the cut streams (S) is expressed as follows.

$$S = \sum_{i=1}^{m} W_i$$

where m is the number of cut streams.

2. Decomposition algorithm

Based on the proposed tearing criteria, an efficient decomposition algorithm is developed as shown in **Fig. 1**, in which selecting the alternative stream with minimum weight is the key point after each cycle interval is detected. The procedures for each step are explained as follows.

Step 1. Cycle interval detecting

The first step of the proposed algorithm is to ensure the minimum number of cut streams (cycle intervals). The weighed reachable vector method is proposed for the detection of cycle intervals, in which the weighed adjacency matrix of the system is used to obtain better initial vertices sequence than non-weighed one.

First, input the weighed adjacency matrix of the system, then constitute the initial vertices sequence according to the order of δ. From the second vertex of the initial sequence, check each vertex one by one to see whether there exists a counter stream in the similar manner of non-weighed adjacency matrix[9]). If there is a counter stream (constituting a cycle interval), write down the local weighed adjacency matrix $\boldsymbol{P}$ corresponding to the counter stream

```
          Step 1
Constitute initial vertex sequence.
Examine counter stream from the
second vertex to n-th vertex.
Detecting cycle accords with the
weighed reachable vector operation
          ↓
          Step 2
When a cycle (a counter stream) is
detected, searching the effective
cut stream with minimum weight
based on the local weighed adjacency
matrix    ↓
          Step 3
Judging is carried out by verifying
whether the detected cycle is broken
or not    ↓
          Step 4
Regulating is implemented to try the
other stream with minimum weight.
Repeat steps 2-4 until the last dete-
cted. Finally the optimal cut-set is
obtained  ↓
          Step 5
Find Boolean sum and final and starting
vertices sequence, constitute calcu-
lation precedence
          ↓
          Stop
```

Fig. 1. The proposed algorithm

interval.

An example named the Forder & Hutchison Digraph[2)] is shown in **Fig. 2**, where figures of the streams indicate the corresponding weights. The following weighed adjacency matrix can be got based on the digraph, where the calculation of in- or out-degree considers the weight of each stream as shown in δ^+ and δ^- respectively.

$$
\begin{array}{cc}
 & \begin{array}{cccccc} A & B & C & D & E & F \end{array} \quad \delta^- \\
A=\begin{array}{c} A \\ B \\ C \\ D \\ E \\ F \end{array} & \left[\begin{array}{cccccc}
0 & 4 & 0 & 0 & 0 & 0 \\
5 & 0 & 8 & 0 & 0 & 0 \\
4 & 0 & 0 & 10 & 0 & 0 \\
6 & 0 & 0 & 0 & 2 & 4 \\
0 & 3 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0
\end{array}\right] \begin{array}{c} 4 \\ 13 \\ 14 \\ 12 \\ 5 \\ 2 \end{array} \\
\delta^+ & \begin{array}{cccccc} 15 & 7 & 10 & 10 & 4 & 4 \end{array} \\
\delta & \begin{array}{cccccc} -11 & 6 & 4 & 2 & 1 & -2 \end{array}
\end{array}
$$

In order of decreasing δ $(=\delta^- - \delta^+)$, the initial vertices sequence, which is BCDEFA, is formed first. Then E→B is detected as a counter stream where the interval is BCDE ($k=4$, k is the length of the counter stream interval). The local weighed adjacency matrix is

$$
\boldsymbol{P}=\begin{bmatrix} 0 & 8 & 0 & 0 \\ 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 2 \\ 3 & 2 & 0 & 0 \end{bmatrix}
$$

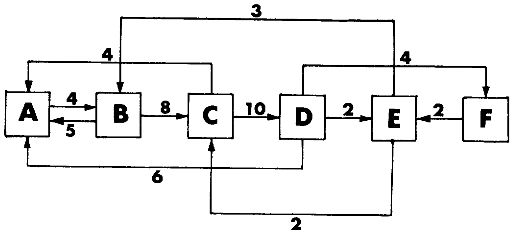

Fig. 2. Forder & Hutchison Digraph (1969)

After the cycle interval is detected, the alternative stream with minimum weight is selected through the following steps.

Step 2. Searching

Based on the principle of graph theory and linear algebra, the alternative stream with minimum weight for each detected cycle interval is searched by the following procedures.

Calculate the weighed reachable vectors using the formula $\boldsymbol{V}^i=\boldsymbol{V}^{i-1}\boldsymbol{P}$ where $\boldsymbol{V}^0=(1, 0, \cdots, 0)$, and check the value of the last element $V^i(k)$. If $V^i(k)=0$ for $i=1, 2, \cdots, k-1$, it is shown that there is no cycle in the counter interval; then turn to procedure Step 5. If $V^i(k)$ is not equal to zero, it indicates that there is an i-step path from the final to the start vertex, and the counter stream must belong to the cycle that consists of $i+1$ streams. Then search the effective cut stream with minimum weight. First, let $p_{\min}=P(k, 1)$ (the weight of the counter stream). Second, search the element $P(i, j)$ from the non-zero elements above the main diagonal line of $\boldsymbol{P}$ which satisfies the following inequality formula:

$$
P(i, j)<p_{\min} \qquad i<j, \\
i=1, 2, \cdots, k-1, \quad j=2, 3, \cdots, k
$$

Then assume $P(i, j)=0$ (the stream is cut), and calculate $\boldsymbol{V}^i$.

In the previous example, because $\boldsymbol{V}^1=(0, 8, 0, 0)$, $\boldsymbol{V}^2=(0, 0, 80, 0)$, $\boldsymbol{V}^3=(0, 0, 0, 160)$, $V^3(4)$ is not equal to zero, it indicates that there is a 3-step cycle. First, let $p_{\min}=P(4, 1)=3$. Then find an element $P(3, 4)=2$ $(<p_{\min})$ corresponding to the stream D→E.

After searching an alternative stream with minimum weight, it is necessary to judge whether it is an effective cut stream.

Step 3. Judging

Based on the weighed reachable vector operation, judging is carried out by verifying whether the detected cycle interval is broken or not. There are two possible cases. For the first case, if $V^i(k)$ is not equal to zero, there exists a cycle. So the stream corresponding to $P(i, j)$ cannot break the detected cycle interval.

For the second case, if $V^i(k)=0$, $i=0, 1, \cdots, k-1$, it indicates that the cut stream corresponding to $P(i, j)$ can break all the cycles in the interval.

According to the cases of the judging result, it is necessary to regulate the corresponding value of the local weighed adjacency matrix for searching the other alternative stream with minimum weight.

In the example, assume that the stream corresponding to $P(3, 4)$ is cut, and calculate the weighed reachable vector $V^1=(0, 8, 0, 0)$, $V^2=(0, 0, 80, 0)$, $V^3=(0, 0, 0, 0)$. Because $V^i(k)=0$ for $i=0, 1, 2, 3$, it indicates that D→E is an effective cut stream.

Step 4. Regulating

Regulating is carried out according to the individual case. For the case of $V^i(k)\neq 0$, regulation is implemented to restore the value of $P(i, j)$. Then the next non-zero element that satisfies the inequality formula is searched continuously. Repeat Steps 2–4 until the element $P(k-1, k)$ is examined. Finally the stream corresponding to $p_{\min}$ is determined as the cut stream. For the case of $V^i(k)=0$, determine $P_{\min}=P(i, j)$.

If the stream corresponding to $p_{\min}$ is not the counter stream detected before, the vertices of this counter stream interval should be reordered to remove all the cycles in the detected cycle interval. Reordering is implemented by assigning the element $P(i, j)$ $(=p_{\min})$ of the local weighed adjacency matrix to zero and going to Step 5.

Up to now, the cut stream with minimum weight is determined for each detected cycle interval. It is then necessary to reorder the sequence for detecting the other cycle interval or determining the feasible calculation precedence in the following step.

In this example, because there is not a non-zero element above the main diagonal line of $\boldsymbol{P}$ that satisfies $P(i, j)<p_{\min}$, assign $P(3, 4)=0$ in $\boldsymbol{P}$, which indicates stream D→E with the minimum weight 2 to be cut.

Because stream D→E is not the counter stream detected before, then reordering must be implemented according to Step 5.

Step 5. Determining calculation precedence

This step is important for reordering the sequence and determining the calculation precedence, which is implemented by the following procedures based on the operation rule of Boolean algebra.

Find the Boolean sum ($\boldsymbol{VS}$) of $V^0, V^1, \cdots, V^{k-1}$, then examine each element of vector $\boldsymbol{VS}$, look for final vertices and start a vertices sequence, and finally join the start vertices sequence with the final vertices sequence to turn a counter stream into a direct stream[9].

In the example, reordering is implemented. Because $\boldsymbol{VS}=(1, 8, 80, 0)$, the final vertices sequence is BCD and the start vertices sequence is E. The interval sequence after adjustment is EBCD, and the initial sequence is changed into EBCDFA.

Determine some alternative stream as a cut stream by Steps 2–4 and change the corresponding element of $\boldsymbol{P}$ to zero. If the cut stream is not the counter stream detected before, arrange the interval sequence into a direct stream according to Step 5, then turn to Step 1 until all vertices ahead of the n-th vertex are checked and disposed. Then the $(n+1)$-th vertex in the sequence is examined. After all vertices are processed, the cut-set and the feasible calculation precedence are determined.

3. Example problems

3.1 Illustration of the proposed algorithm

To illustrate the details of the proposed algorithm, the previous example is continuously decomposed in this section. According to the algorithm proposed in section 2, the initial sequence has changed into EBCDFA. F→E is detected as a counter stream and the interval is EBCDF ($k=5$). The local weighed adjacency matrix is

$$\boldsymbol{P}=\begin{bmatrix} 0 & 3 & 2 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 4 \\ 2 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Then $V^1=(0, 3, 2, 0, 0)$, $V^2=(0, 0, 24, 20, 0)$, $V^3=(0, 0, 0, 240, 80)$. Because $V^3(5)=80$ is not equal to zero, it indicates that there is a 3-step cycle. First let $p_{\min}=P(5, 1)=2$. Then searching is carried out. There is not a non-zero element above main diagonal line of $\boldsymbol{P}$ satisfying $P(i, j)<p_{\min}$, so assign $P(5, 1)=0$ in $\boldsymbol{P}$, which indicates that stream F→E with the minimum weight 2 is to be cut.

A→B is a counter stream and the interval is BCDFA ($k=5$). The local weighed adjacency matrix is

$$\boldsymbol{P}=\begin{bmatrix} 0 & 8 & 0 & 0 & 5 \\ 0 & 0 & 10 & 0 & 4 \\ 0 & 0 & 0 & 4 & 6 \\ 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and $V^1=(0, 8, 0, 0, 5)$. Then there is a 1-step cycle. Let $p_{\min}=P(5, 1)=4$, and carry out searching. There is not a non-zero element $P(i, j)$ which satisfies $P(i, j)<p_{\min}$, so $p_{\min}=P(5, 1)=4$. The stream A→B is determined as the cut stream with minimum weight 4. The examination of the initial vertices sequence is now finished. The cut-set and the calculation precedence are obtained as {D→E; F→E; A→B} with the weighing sums 8 and EBCDFA respectively.

If the adjacency matrix of the system is used instead of the weighed one, the obtained initial vertices sequence will be DBCEFA. Then, using the proposed algorithm, after one selection cycle (searching, judging and regulating) the initial vertices sequence will turn to the sequence BCDEFA, which is just the initial sequence determined by the weighed adjacency matrix. Therefore, using the weighed adjacency matrix of the system is efficient in the algorithm.

3.2 Comparison of results

To illustrate the effectiveness of the proposed algorithm, some algorithms used for the weighed process decomposition are compared in finding out the cut-set of **Fig. 3**, where figures indicate the corresponding streams henceforth. According to the general knowledge of iterative convergence, the first basis of comparison is the number of cut streams and the second basis is the weighing sum of the cut streams. To compare the proposed algorithm with M & H-2, this study also takes the same scheme of assigning weight with M & H-2, in which the weight of each stream is equal to the number of output streams of that node. The cut-sets obtained by other algorithms are given in **Table 1**, and it is clear that the proposed algorithm produces the best cut-set (minimum weighing sum) with the same number of cut streams.

Similarly, the cut-sets obtained by the previous algorithms for two more digraphs, as shown in **Figs. 4** and **5** are summarized in **Table 2**, which indicates that the proposed and M & H-2 algorithms in these cases perform equally well.

Finally, the cut-sets are evaluated for a relatively complicated digraph of a sulfuric acid plant which possesses 44 units and 69 streams, shown in **Fig. 6**. The results are shown in **Table 3**. Using the proposed algorithm the minimum number of cut streams can be got; at the same time the weighing sum of the cut-set is also minimum.

In these Tables, NC^* indicates the number of cut streams and S^{**} represents the weighing sum of the cut-set.

From the above results, it is shown that the proposed algorithm can always find out the optimal cut-set (minimum weighing sum with minimum number of cut streams) compared with the other decomposition algorithms.

Conclusion

For decreasing the computation load, it is proposed as tearing criteria that the number of cut streams be minimized first and then an alternative stream with minimum weight be searched for each detected cycle interval. Based on them, an algorithm is newly developed for weighed process decomposition. In the proposed algorithm, after detecting a cycle interval, an effective cut stream with minimum weight is searched on the local weighed adjacency matrix first. Then judging is carried out by verifying whether the detected cycle interval is broken or not. Finally, regulating is implemented to find the other alternative stream with minimum weight. Searching, judging and regulating are repeated until the optimal cut-set is got. Through four examples, it is shown

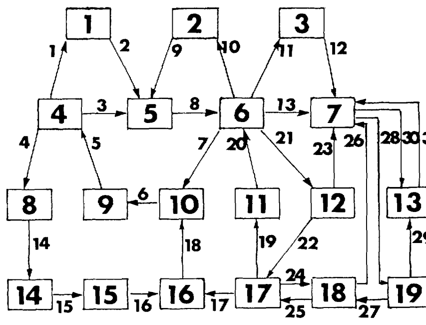

Fig. 3. Sargent & Westerberg Digraph (1964)

Table 1. Comparison of results for Fig. 3

Algorithm	cut-set	NC^*	S^{**}
BTA[5]	8, 18, 22, 25, 27, 31	6	16
K & S[6]	5, 8, 20, 25, 28, 31	6	20
M & H-2[7]	6, 10, 21, 24, 28, 30	6	9
This study	7, 10, 18, 25, 28, 30	6	8

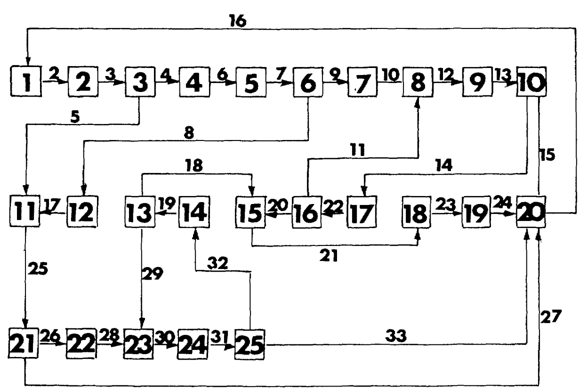

Fig. 4. Christensen & Rudd Digraph (1969)

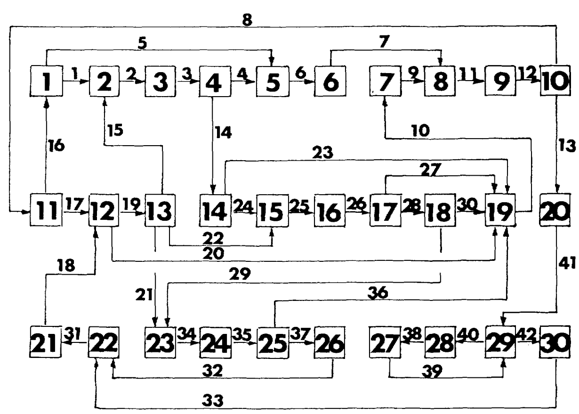

Fig. 5. Christensen & Rudd Digraph (1969)

Table 2. Comparison of results for Figs. 4 and 5

Algorithm	Digraph, Fig. 4 cut-set	S^{**}	Digraph, Fig. 5 cut-set	S^{**}
BTA[5]	16, 22, 31	5	12, 35, 40	5
K & S[6]	3, 13, 31	6	12, 19, 39	7
M & H-2[7]	12, 16, 32	3	11, 34, 40	3
This study	12, 16, 30	3	11, 34, 40	3

Table 3. Cut-sets for sulfuric acid plant, Fig. 6

Algorithm	cut-set	NC^*	S^{**}
BTA[5])	18, 25, 32 38, ,40, 43 58, 63, 64	9	13
M & H-2[6]	13, 16, 31 46, 58, 60	6	10
This study	14, 31, 45, 58, 60	5	9

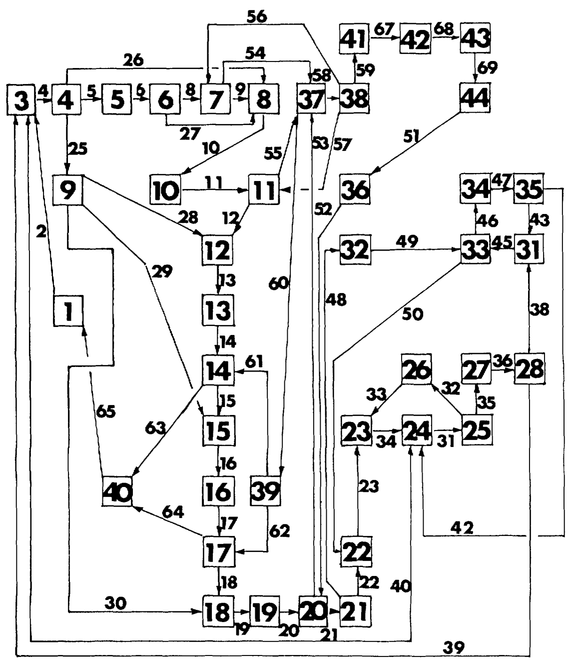

Fig. 6. Sulfuric Acid Plant Digraph (1971)

that the proposed algorithm is a much more effective method compared with other decomposition algorithms for weighed processes.

Nomenclature

A	=	initial weighed system adjacency matrix
$A(i, j)$	=	element of initial weighed system adjacency matrix
I	=	number of vertices
k	=	dimension of local adjacency matrix or element number of reachable vector
l	=	number of effective cut streams in the counter stream interval
m	=	number of cut streams
$\boldsymbol{P}$	=	k dimension local weighed adjacency matrix
$P(i, j)$	=	element of local weighed adjacency matrix
S	=	weighting sum of cut streams
$\cup$	=	Boolean sum or logical sum
$\boldsymbol{V}$	=	reachable vector
$V(i)$	=	element of reachable vector
$\boldsymbol{VS}$	=	result vector of Boolean sum
W_i	=	minimum weight of the i-th cycle
$\delta(v)$	=	degree of vertex

⟨Superscripts⟩

i	=	step number of reachable vector
$+$	=	in-degree of vertex
$-$	=	out-degree of vertex

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