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Application of Partitioning and Tearing Techniques to Sulfolane Extraction Plant

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Abstract–For effective flowsheet-level calculation of a complex chemical plant, the use of suitable partitioning and tearing techniques is inevitable. The partitioning and tearing techniques based on the reachability matrix and the decomposition algorithm were applied to model and simulate a sulfolane extraction plant. Basic concepts were first exploited towards a general representation for the modeling and simulation of the sulfolane extraction process. Six process units, which consist of the sulfolane extraction plant, were modeled first and partitioning and tearing techniques were employed to model and simulate the whole extraction plant. The Inside-Out method and the sequential-modular approach were used in the modeling and simulation. Results of simulations showed good agreement with plant operation data.

Key words : Sulfolane Extraction, Partitioning, Tearing, Decomposition Algorithm

INTRODUCTION

The sulfolane extraction process is widely used in benzene-toluene-xylene (BTX) plants to separate aromatics from the hydrotreated feedstocks. Operation of the sulfolane process affects essentially the overall efficiency of BTX plants. This paper proposes a computational tool for an industrial sulfolane extraction process, which can be used to analyze and optimize operation and design of the process. In the sulfolane extraction process considered in the present study benzene, toluene, xylene and C_9 aromatics are recovered from aromatic-rich depentanized streams. The sulfolane extraction process considered in this work consists of the extraction section and the fractionation section. The extraction section consists of an extractor, an extractive distillation and a recovery column as shown in Fig. 1.

The whole process consists of six columns and two settlers. The aromatics are extracted from the feedstock in the extraction section of the unit and are recovered separately in the associated fractionation section. The product purity and recovery efficiency in the liquid-liquid extraction and distillation processes depend on the solubility and selectivity characteristics of sulfolane for various types of hydrocarbons. Sulfolane has high selectivity for aromatics, high solubility for water and high boiling point [Bailes and Hughes, 1976]. Non-aromatic hydrocarbons remaining in the rich solvent are removed in the stripper column and recycled to the extractor as can be seen in Fig. 1. A water-stripping column is provided to remove traces of dissolved non-aromatics from the solvent-rich wash water and to generate stripping steam for the recovery column.

Among four unit plants comprising a BTX plant, the sulfolane extraction plant is by far the most important unit. The economics and operational stability of a BTX plant are heavily dependent on the operation status of the sulfolane extraction plant. Therefore, the development and use of a simulation system for the sulfolane extraction plant will be very helpful to identify optimal operating conditions and to increase product quality. To date, the authors have not found any modeling and simulation results concerning the sulfolane extraction plant.

For effective flowsheet-level calculation, suitable partitioning and tearing are inevitable. Various tearing algorithms [Upadhye and Grens, 1975; Genna and Motard, 1975] are available and the decomposition algorithm [Ollero and Amselem, 1983] is applied in the present study. Most of these methods can be classified into three types : simplification of the digraph based on local structures, techniques based on a cycle matrix, and implicit enumeration. In digraph simplification techniques edges are eliminated and vertices are aggregated without changing the cycle structure and the number of tears in the digraph. In terms of a cycle matrix a tear set is a set of edges whose union contains a nonzero in each cycle of the matrix. An optimal algorithm usually requires the generation of all circuits, which can be quite demanding in computing time and memory. In the implicit enumeration technique dynamic programming and branch and bound methods have been applied. This method guarantees a minimal tear set, but it is limited by the dimensionality of the problem considered. Among many numerical methods [Crowe and Nishio, 1975; Motard et al., 1975] available to compute the flowsheet-level problem, we employed the direct substitution method [Metcalfe and Perkins, 1978].

The plant considered in the present study is the sulfolane extraction plant now being operated in Daelim Petrochemical Co. located in the southwestern area of Korea. The main purpose of the present work is to show how the partitioning and tearing techniques can be applied to the actual plant and how the actual operation can benefit from the computational techniques. Because of the lack of published results on modeling and simulation of the sulfolane extraction plant, we first analyzed the

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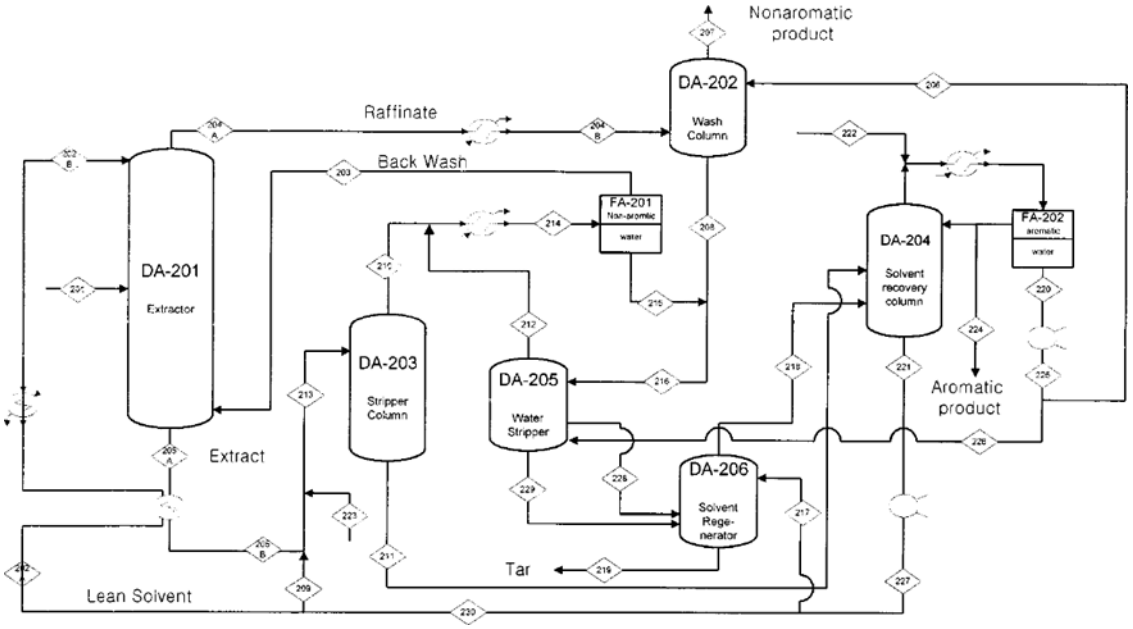

Fig. 1. The flowsheet of the sulfolane extraction process.

operation data and the flowsheet of the plant as well as the heuristic operational knowledge of the plant engineers. Results of computations were compared to operation data to verify the effectiveness and usefulness of the present work. Details on the computations of each process unit are not shown in this paper. Those who are interested in the modeling and simulation of each process unit can refer to the published result [Choo et al., 1998].

PARTITIONING

For efficient flowsheeting we have to identify the strong component in the digraph (directed graph) through partitioning. The digraph of the sulfolane extraction process being considered is shown in Fig. 2. Partitioning operation reduces the number of processing units or equations which must be considered simultaneously at any time. For partitioning operation we usually employ the graphical representation of the process flowsheet using nodes and directed edges. In general nodes represent units and junctions and the matrix which describes the relationship between nodes is called the node adjacency matrix. The (i, j)th element of the matrix is assigned a nonzero value (typically "1") if there is a directed edge from node i to node j, otherwise zero. The node adjacency matrix for the sulfolane extraction process being considered is shown in Table 1.

Reachability matrix is obtained from the node adjacency matrix. In the reachability matrix,

(1) The (i, j)th element of $\mathbf{X}^k$ gives the number of **k**-step edge sequences from node i to node j.

(2) For an acyclic digraph $\mathbf{k}^{k+m}=\mathbf{0}$, where $\mathbf{m}>\mathbf{0}$ and $\mathbf{k}\geq\mathbf{N}-1$, **k** being the longest path in the digraph.

(3) For a cyclic digraph nonzero elements appear and disappear on the digraph as the power increases. In fact, as power of **X** increases, it becomes periodic.

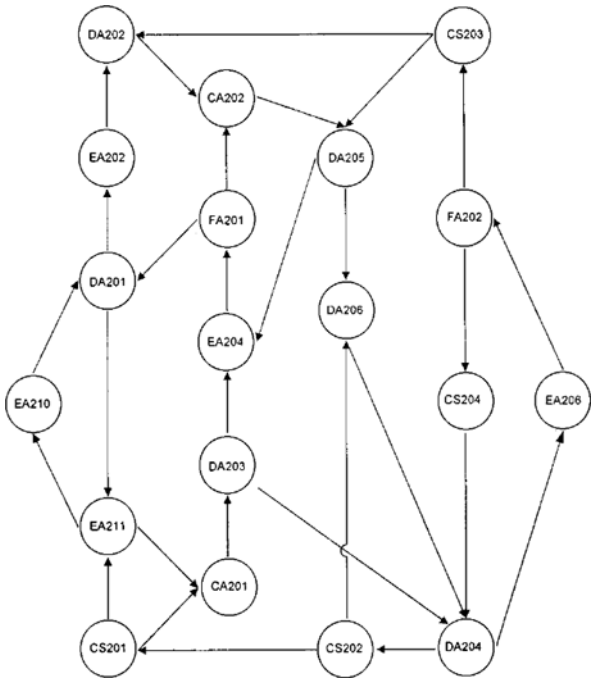

Fig. 2. The digraph of the sulfolane extraction process.

Let us define the Boolean equivalent of any matrix **B** as

$$\mathbf{B}_{ij}^{\#}=\begin{cases}\mathbf{0}, & \text{if } \mathbf{b}_{ij}=\mathbf{0}\\ \mathbf{1}, & \text{if } \mathbf{b}_{ij}\neq\mathbf{0}\end{cases}$$

The Boolean equivalent of the sum of the first **N** powers of **X**, the reachability matrix

$$\mathbf{R}=(\mathbf{X}+\mathbf{X}^2+\mathbf{X}^3+\cdots+\mathbf{X}^N)^{\#}$$

is a special matrix whose (i, j)th element indicates whether there exists any directed path of any length from node i to node j. The

Table 1. Node adjacency matrix of the sulfolane extraction proces

	EA210	DA201	EA202	DA202	CA202	FA201	EA204	DA203	EA211	CA201
EA210		1								
DA201			1						1	
EA202				1						
DA202					1					
CA202										
FA201		1			1					
EA204						1				
DA203							1			
EA211	1									1
CA201								1		
CS201									1	1
CS202										
DA206										
DA205							1			
DA204										
EA206										
FA202										
CS204										
CS203				1						

	CS201	CS202	DA206	DA205	DA204	EA206	FA202	CS204	CS203
EA210									
DA201									
EA202									
DA202									
CA202				1					
FA201									
EA204									
DA203					1				
EA211									
CA201									
CS201									
CS202	1		1						
DA206					1				
DA205			1						
DA204		1				1			
EA206							1		
FA202								1	1
CS204					1				
CS203				1					

maximal cyclic blocks, or strong components of the digraph, are obtained by the intersection of **R** and its transpose. The reachability matrix of the sulfolane extraction process being considered is shown in Table 2. As shown in Table 2, the whole extraction process consists of only one strong component. For this reason, the values of unit modules of the whole process are calculated and those of each stream need to be updated at each iteration stage. The sequential-modular approach is applied because each unit module is not iterated.

TEARING

For the efficient partitioning computation, specific stream(s) to be guessed should be chosen carefully. In this paper, the decomposition algorithm by Ollero and Amselem [1983] is applied for the decision of the stream(s) being guessed. The algorithm is well known to be simple and fast for minimizing the number of tear streams [Mah, 1990]. The relationship between streams can be described by a stream adjacency matrix. In a stream adjacency matrix, the edges are represented by the rows and the columns. The (i, j)th element is assigned a nonzero value (typically "1") if edge i is headed into a node and edge j comes out of the same node.

The stream adjacency matrix of the sulfolane extraction process being considered is shown in Table 3. The set of all the immediate successors to the node n is denoted by T(n) and the set of all the immediate predecessors to n is denoted by $T^{-1}(n)$. The decomposition algorithm requires two simple graph operations: non-essential stream node reduction and essential stream node reduction. In the non-essential stream node reduction the stream node n_i is deleted from the signal flowgraph and the set of nodes in $T^{-1}(n_i)$ is connected to the set of nodes in $T(n_i)$. In the essential stream node reduction node n_q and all the edges connected to it are deleted from the signal flow graph. Two possible situations can arise as a result of repeated applications of non-essential stream node reduction: the appearance of nodes with a self-loop

Table 2. Reachability matrix of the sulfolane extraction process

	EA210	DA201	EA202	DA202	CA202	FA201	EA204	DA203	EA211
EA210	1	1	1	1	1	1	1	1	1
DA201	1	1	1	1	1	1	1	1	1
EA202	1	1	1	1	1	1	1	1	1
DA202	1	1	1	1	1	1	1	1	1
CA202	1	1	1	1	1	1	1	1	1
FA201	1	1	1	1	1	1	1	1	1
EA204	1	1	1	1	1	1	1	1	1
DA203	1	1	1	1	1	1	1	1	1
EA211	1	1	1	1	1	1	1	1	1
CA201	1	1	1	1	1	1	1	1	1
CS201	1	1	1	1	1	1	1	1	1
CS202	1	1	1	1	1	1	1	1	1
DA206	1	1	1	1	1	1	1	1	1
DA205	1	1	1	1	1	1	1	1	1
DA204	1	1	1	1	1	1	1	1	1
EA206	1	1	1	1	1	1	1	1	1
FA202	1	1	1	1	1	1	1	1	1
CS204	1	1	1	1	1	1	1	1	1
CS203	1	1	1	1	1	1	1	1	1

	CA201	CS201	CS202	DA206	DA205	DA204	EA206	FA202	FA202	CS204	CS203
EA210	1	1	1	1	1	1	1	1	1	1	1
DA201	1	1	1	1	1	1	1	1	1	1	1
EA202	1	1	1	1	1	1	1	1	1	1	1
DA202	1	1	1	1	1	1	1	1	1	1	1
CA202	1	1	1	1	1	1	1	1	1	1	1
FA201	1	1	1	1	1	1	1	1	1	1	1
EA204	1	1	1	1	1	1	1	1	1	1	1
DA203	1	1	1	1	1	1	1	1	1	1	1
EA211	1	1	1	1	1	1	1	1	1	1	1
CA201	1	1	1	1	1	1	1	1	1	1	1
CS201	1	1	1	1	1	1	1	1	1	1	1
CS202	1	1	1	1	1	1	1	1	1	1	1
DA206	1	1	1	1	1	1	1	1	1	1	1
DA205	1	1	1	1	1	1	1	1	1	1	1
DA204	1	1	1	1	1	1	1	1	1	1	1
EA206	1	1	1	1	1	1	1	1	1	1	1
FA202	1	1	1	1	1	1	1	1	1	1	1
CS204	1	1	1	1	1	1	1	1	1	1	1

and the presence of stream nodes with no inputs and outputs. The nodes with a self-loop are deleted by means of the essential reduction and must be members of the minimum tear set since there is no alternative which will reduce cyclicity. The stream nodes with no inputs and outputs cannot be the member of the minimum tear set. But they can also be deleted by means of the essential stream node reduction.

MODELING EQUATIONS

Based on the results of partitioning and tearing described before, the whole flowsheet can now be computed. The diagram of unit modules and streams is shown in Fig. 3. The model equations of each unit module can be represented as follows. In these equations each variable is a vector that represents temperature and composition. The inside-out method [Boston and Sullivan, 1974] was used in the modeling and simulation of each process unit. Details on the modeling equations and thermodynamical relations are shown elsewhere [Choo et al., 1998].

- Separator

$$f_1(\mathbf{I}_1, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_{13})=\mathbf{0} \begin{cases} \mathbf{x}_2=\mathbf{f}_1(\mathbf{I}_1, \mathbf{x}_1, \mathbf{x}_{13}) \\ \mathbf{x}_3=\mathbf{f}_{12}(\mathbf{I}_1, \mathbf{x}_1, \mathbf{x}_{13}) \end{cases} \quad (1)$$

$$f_2(\mathbf{x}_{15}, \mathbf{x}_{16}, \mathbf{x}_{30}, \mathbf{x}_{31})=\mathbf{0} \begin{cases} \mathbf{x}_{16}=\mathbf{f}_{21}(\mathbf{x}_{15}, \mathbf{x}_{30}) \\ \mathbf{x}_{31}=\mathbf{f}_{22}(\mathbf{I}_{15}, \mathbf{x}_{30}) \end{cases} \quad (2)$$

$$f_3(\mathbf{x}_9, \mathbf{x}_{10}, \mathbf{x}_{11})=\mathbf{0} \begin{cases} \mathbf{x}_{10}=\mathbf{f}_{31}(\mathbf{x}_{\cdot} \\ \mathbf{x}_{31}=\mathbf{f}_{32}(\mathbf{x}_{\cdot} \end{cases} \quad (3)$$

$$f_4(\mathbf{x}_1, \mathbf{x}_{22}, \mathbf{x}_{23}, \mathbf{x}_{24}, \mathbf{x}_{27})=\mathbf{0} \begin{cases} \mathbf{x}_{23}=\mathbf{f}_{41}(\mathbf{x}_{10}, \mathbf{x}_{22}, \mathbf{x}_{27}) \\ \mathbf{x}_{24}=\mathbf{f}_{42}(\mathbf{x}_{10}, \mathbf{x}_{22}, \mathbf{x}_{27}) \end{cases} \quad (4)$$

Table 3. Stream adjacency matrix of the sulfolane extraction process

	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}	X_{11}	X_{12}	X_{13}	X_{14}	X_{15}
X_1		1	1												
X_2															1
X_3				1		1									
X_4									1						
X_5				1		1									
X_6	1														
X_7									1						
X_8					1		1								
X_9										1	1				
X_{10}															
X_{11}												1			
X_{12}													1	1	
X_{13}		1	1												
X_{14}															
X_{15}															
X_{16}															
X_{17}															
X_{18}												1			
X_{19}															
X_{20}															
X_{21}															
X_{22}															
X_{23}															
X_{24}								1							
X_{25}															
X_{26}															
X_{27}															
X_{28}															
X_{29}															
X_{30}															

	X_{16}	X_{17}	X_{18}	X_{19}	X_{20}	X_{21}	X_{22}	X_{23}	X_{24}	X_{25}	X_{26}	X_{27}	X_{28}	X_{29}	X_{30}
X_1															
X_2															
X_3															
X_4															
X_5															
X_6															
X_7															
X_8															
X_9															
X_{10}								1	1						
X_{11}															
X_{12}															
X_{13}															
X_{14}		1													
X_{15}	1														
X_{16}		1													
X_{17}			1	1	1										
X_{18}															
X_{19}							1								
X_{20}							1								
X_{21}							1								
X_{22}								1	1						
X_{23}										1					
X_{24}						1									
X_{25}											1		1		
X_{26}												1			
X_{27}								1	1						
X_{28}														1	1
X_{29}			1	1	1										
X_{30}	1														

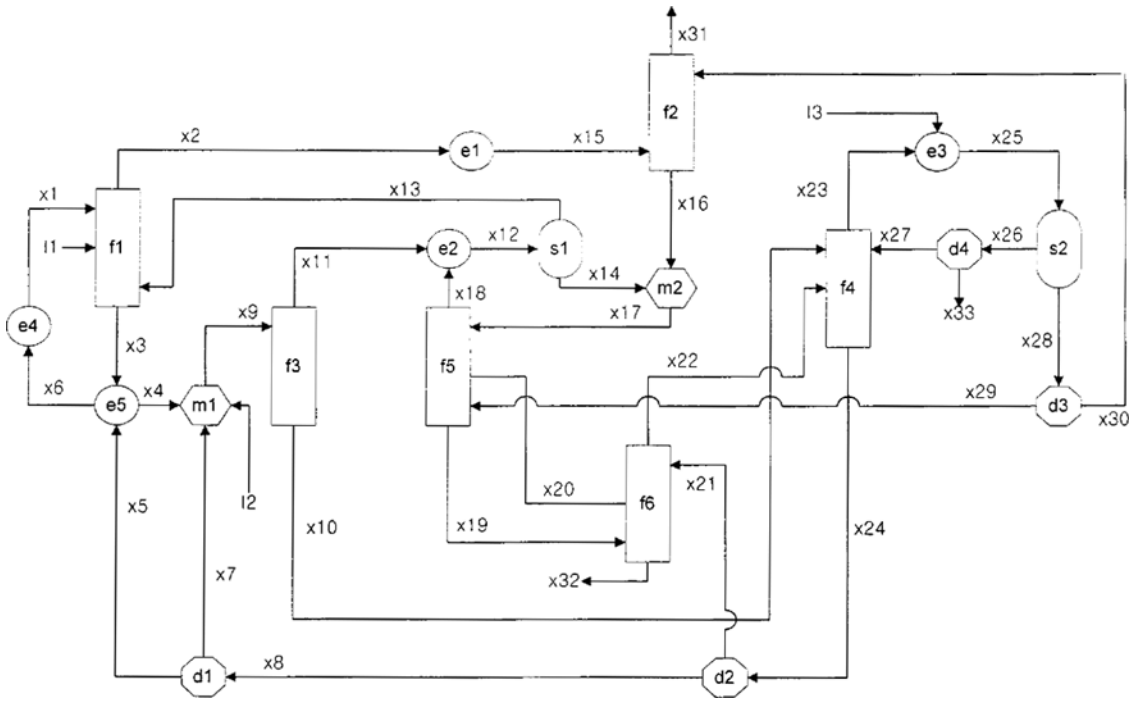

Fig. 3. The diagram of unit modules and streams.

$$\mathbf{f}_5(\mathbf{x}_{17},\ \mathbf{x}_{18},\ \mathbf{x}_{19},\ \mathbf{x}_{20},\ \mathbf{x}_{29})=\mathbf{0}\begin{cases}\mathbf{x}_{18}=\mathbf{f}_{51}(\mathbf{x}_{17},\ \mathbf{x}_{29})\\ \mathbf{x}_{19}=\mathbf{f}_{52}(\mathbf{x}_{17},\ \mathbf{x}_{29})\\ \mathbf{x}_{20}=\mathbf{f}_{53}(\mathbf{x}_{17},\ \mathbf{x}_{29})\end{cases} \quad (5)$$

$$\mathbf{f}_6(\mathbf{x}_{19},\ \mathbf{x}_{20},\ \mathbf{x}_{21},\ \mathbf{x}_{22},\ \mathbf{x}_{32})=\mathbf{0}\begin{cases}\mathbf{x}_{22}=\mathbf{f}_{61}(\mathbf{x}_{19},\ \mathbf{x}_{20},\ \mathbf{x}_{21})\\ \mathbf{x}_{32}=\mathbf{f}_{62}(\mathbf{x}_{19},\ \mathbf{x}_{20},\ \mathbf{x}_{21})\end{cases} \quad (6)$$

• Settler

$$\mathbf{s}_1(\mathbf{x}_{12},\ \mathbf{x}_{13},\ \mathbf{x}_{14})=\mathbf{0}\begin{cases}\mathbf{x}_{13}=\mathbf{s}_1(\mathbf{x}_{12})\\ \mathbf{x}_{14}=\mathbf{s}_{12}(\mathbf{x}_{12})\end{cases} \quad (7)$$

$$\mathbf{s}_2(\mathbf{x}_{25},\ \mathbf{x}_{26},\ \mathbf{x}_{28})=\mathbf{0}\begin{cases}\mathbf{x}_{26}=\mathbf{s}_{21}(\mathbf{x}_{25})\\ \mathbf{x}_{28}=\mathbf{s}_{22}(\mathbf{x}_{25})\end{cases} \quad (8)$$

• Divider

$$\mathbf{d}_1(\mathbf{x}_5,\ \mathbf{x}_7,\ \mathbf{x}_8)=\mathbf{0}\begin{cases}\mathbf{x}_5=\mathbf{d}_{11}(\mathbf{x}_8)\\ \mathbf{x}_7=\mathbf{d}_{12}(\mathbf{x}_8)\end{cases} \quad (9)$$

$$\mathbf{d}_2(\mathbf{x}_8,\ \mathbf{x}_{21},\ \mathbf{x}_{24})=0\begin{cases}\mathbf{x}_8=\mathbf{d}_{21}(\mathbf{x}_{24})\\ \mathbf{x}_{21}=\mathbf{d}_{22}(\mathbf{x}_{24})\end{cases} \quad (10)$$

Table 4. Tearing variable condition for design data

		x_3 (205A)	x_{17} (216)	x_{24} (221)	x_{25} (222B)
Flowrate (ton/hr)					
	Cyclopentane	3.66287	0.00021	0.00000	0.00000
	Hexane	0.08394	0.00017	0.00000	0.00000
	Methylcyclopen	6.66621	0.00042	0.00031	0.00000
	Benzene	11.81168	0.00023	0.00000	14.32282
	3-Methylhexane	0.00548	0.00000	0.00000	0.00000
	Methylcyclohex	0.91169	0.00010	0.00000	0.00000
	Toluene	6.20779	0.00000	0.00000	8.44658
	Octane	0.00046	0.00000	0.00000	0.00000
	DMCH	0.01077	0.00000	0.00000	0.01414
	Ethylbenzene	1.92580	0.00000	0.00000	2.69475
	p-Xylene	0.42488	0.00000	0.00000	0.52565
	m-Xylene	1.20873	0.00000	0.00000	1.36961
	o-Xylene	0.43858	0.00000	0.00000	0.10434
	Sulfolane	108.51075	0.09553	156.97156	0.00000
	Water	0.68461	2.34906	0.94737	4.22939
Temperature (°C)		56.20000	41.50000	180.20000	40.00000

Table 5. The comparison of design data and simulation results

		205A		213		216		221	
Flowrate (ton/hr)		Design	Calculation	Design	Calculation	Design	Calculation	Design	Calculation
	Cyclopentane	3.66287	3.95496	3.67851	3.80546	0.00021	0.00001	0.00000	0.00000
	Hexane	0.08394	0.05724	0.08394	0.06847	0.00017	0.00000	0.00000	0.00000
	Methylcyclopen	6.66621	7.08969	6.66621	6.85026	0.00042	0.00000	0.00031	0.00000
	Benzene	11.81168	10.41784	11.81176	10.87382	0.00023	0.00000	0.00000	0.00001
	3-Methylhexane	0.00548	0.00222	0.00541	0.00341	0.00000	0.00000	0.00000	0.00000
	Methylcyclohex	0.91169	0.65998	0.91169	0.76527	0.00010	0.00000	0.00000	0.00000
	Toluene	6.20779	5.86521	6.20779	5.97742	0.00000	0.00000	0.00000	0.00000
	Octane	0.00046	0.00011	0.00046	0.00022	0.00000	0.00000	0.00000	0.00000
	DMCH	0.01077	0.00471	0.01077	0.00700	0.00000	0.00000	0.00000	0.00000
	Ethylbenzene	1.92580	1.92141	1.92580	1.96107	0.00000	0.00000	0.00000	0.00110
	p-Xylene	0.42488	0.46556	0.42468	0.45872	0.00000	0.00000	0.00000	0.04620
	m-Xylene	1.20873	1.34650	1.20873	1.28091	0.00000	0.00000	0.00000	0.22096
	o-Xylene	0.43858	0.68701	0.43858	0.56674	0.00000	0.00000	0.00000	0.47897
	Sulfolane	108.51075	108.49271	154.71719	154.71879	0.09553	0.10882	156.97156	156.97919
	Water	0.68461	0.37611	0.96348	0.82411	2.34906	2.62636	0.94737	0.50257
Temperature (°C)		56.20000	56.20000	89.40000	89.19205	41.50000	40.75540	180.20000	183.80712

Table 6. The comparison of operating data (load 100 %) and simulation results

	205A		207		212	
	Operation	Simulation	Operation	Simulation	Operation	Simulation
Temperature (°C)	58.9	58.9	30.6	30.9	116.3	116.04
Flowrate (ton/hr)	152.9	153.8	7.08	11.5	0.1505	0.755
	213		221		224	
	Operation	Simulation	Operation	Simulation	Operation	Simulation
Temperature (°C)	80.6	80.64	168.1	175.02	30.9	30.9
Flowrate (ton/hr)	183	183.37	145.59	150.0	25.1	27.11

$$\mathbf{d}_3(\mathbf{x}_{28},\ \mathbf{x}_{29},\ \mathbf{x}_{30})=\mathbf{0}\quad\begin{cases}\mathbf{x}_{29}=\mathbf{d}_{31}(\mathbf{x}_{28})\\ \mathbf{x}_{30}=\mathbf{d}_{32}(\mathbf{x}_{28})\end{cases}\tag{11}$$

$$\mathbf{d}_4(\mathbf{x}_{26},\ \mathbf{x}_{27},\ \mathbf{x}_{33})=\mathbf{0}\quad\begin{cases}\mathbf{x}_{27}=\mathbf{d}_{41}(\mathbf{x}_{28})\\ \mathbf{x}_{33}=\mathbf{d}_{42}(\mathbf{x}_{26})\end{cases}\tag{12}$$

- Mixer

$$\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{x}_4,\ \mathbf{x}_9,\ \mathbf{x}_7)=\mathbf{0}\quad \mathbf{x}_9=\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{x}_4,\ \mathbf{x}_7)\tag{13}$$

$$\mathbf{m}_2(\mathbf{x}_{14},\ \mathbf{x}_{16},\ \mathbf{x}_{17})=\mathbf{0}\quad \mathbf{x}_{17}=\mathbf{m}_2(\mathbf{x}_{14},\ \mathbf{x}_{16})\tag{14}$$

- Heat Exchanger

$$\mathbf{e}_1(\mathbf{x}_2,\ \mathbf{x}_{15})=\mathbf{0}\quad \mathbf{x}_{15}=\mathbf{e}_1(\mathbf{x}_2)\tag{15}$$

$$\mathbf{e}_2(\mathbf{I}_{1\,s},\ \mathbf{x}_{12},\ \mathbf{x}_{18})=\mathbf{0}\quad \mathbf{x}_{12}=\mathbf{e}_2(\mathbf{x}_{1\,s},\ \mathbf{x}_{18})\tag{16}$$

$$\mathbf{e}_3(\mathbf{I}_3,\ \mathbf{x}_{23},\ \mathbf{x}_{25})=\mathbf{0}\quad \mathbf{x}_{25}=\mathbf{e}_3(\mathbf{I}_3,\ \mathbf{x}_{23})\tag{17}$$

$$\mathbf{e}_4(\mathbf{x}_1,\ \mathbf{x}_6)=\mathbf{0}\quad \mathbf{x}_1=\mathbf{e}_4(\mathbf{x}_6)\tag{18}$$

$$\mathbf{e}_5(\mathbf{x}_3,\ \mathbf{x}_4,\ \mathbf{x}_5,\ \mathbf{x}_6)=\mathbf{0}\begin{cases}\mathbf{x}_4=\mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{x}_5)\\ \mathbf{x}_6=\mathbf{e}_{52}(\mathbf{x}_3,\ \mathbf{x}_5)\end{cases}\tag{19}$$

To reduce further the number of nonlinear equations that must be solved simultaneously, an appropriate subset of connecting streams are torn instead of all connecting streams. Streams that are not torn can be eliminated. Using the above model equations, the computing sequence can be decided based on tearing variables. For the sulfolane extraction process being considered here we have 4 tearing variables ($\mathbf{x}_3$, $\mathbf{x}_{17}$, $\mathbf{x}_{24}$ and $\mathbf{x}_{25}$) obtained from the partitioning and tearing operations described before :

$$\begin{aligned}\mathbf{x}_3=&\mathbf{f}_{12}(\mathbf{I}_1,\ \mathbf{e}_4(\mathbf{e}_{52}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{x}_{24}))),\\ &\mathbf{s}_1(\mathbf{e}_2(\mathbf{f}_{32}(\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{d}_{21}(\mathbf{x}_{24}))))),\\ &\mathbf{f}_{51}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25})))))\\ &=\mathbf{mod}_1(\mathbf{x}_3,\ \mathbf{x}_{17},\ \mathbf{x}_{24},\ \mathbf{x}_{25})\end{aligned}\tag{20}$$

$$\begin{aligned}\mathbf{x}_{17}=&\mathbf{m}_2(\mathbf{s}_1(\mathbf{e}_2(\mathbf{f}_{32}(\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{d}_{21}(\mathbf{x}_{24}))))),\\ &\mathbf{f}_{51}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25})))),\ \mathbf{f}_{21}(\mathbf{e}_1(\mathbf{f}_{11}(\mathbf{I}_1,\ \mathbf{e}_{4\,t}(\mathbf{e}_{52}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{x}_{24}))),\\ &\mathbf{s}_1(\mathbf{e}_2(\mathbf{f}_{32}(\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{d}_{21}(\mathbf{x}_{24}))))),\\ &\mathbf{f}_{51}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25}))))),\ \mathbf{d}_{32}(\mathbf{s}_{22}(\mathbf{x}_{25})))\\ &=\mathbf{mod}_2(\mathbf{x}_3,\ \mathbf{x}_{17},\ \mathbf{x}_{24},\ \mathbf{x}_{25})\end{aligned}\tag{21}$$

$$\begin{aligned}\mathbf{x}_{24}=&\mathbf{f}_{42}(\mathbf{f}_{31}(\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{d}_1(\mathbf{d}_{21}(\mathbf{x}_{24}))),\ \mathbf{d}_{12}(\mathbf{d}_{21}(\mathbf{x}_{24}))),\\ &\mathbf{f}_{61}(\mathbf{f}_{52},\ \mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25}))),\ \mathbf{f}_{53}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25}))),\ \mathbf{d}_{22}(\mathbf{x}_{24})),\\ &\mathbf{d}_{41}(\mathbf{s}_{21}(\mathbf{x}_{25})))\\ &=\mathbf{mod}_3(\mathbf{x}_3,\ \mathbf{x}_{17},\ \mathbf{x}_{24},\ \mathbf{x}_{25})\end{aligned}\tag{22}$$

$$\begin{aligned}\mathbf{x}_{25}=&\mathbf{e}_3(\mathbf{I}_3,\ \mathbf{f}_{41}(\mathbf{f}_{31}(\mathbf{m}_1(\mathbf{I}_2,\ \mathbf{e}_{51}(\mathbf{x}_3,\ \mathbf{d}_{11}(\mathbf{d}_{21}(\mathbf{x}_{24}))),\\ &\mathbf{d}_{12}(\mathbf{d}_{21}(\mathbf{x}_{24})))),\ \mathbf{f}_{61}(\mathbf{f}_{52}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25}))),\\ &\mathbf{f}_{53}(\mathbf{x}_{17},\ \mathbf{d}_{31}(\mathbf{s}_{22}(\mathbf{x}_{25}))),\ \mathbf{d}_{22}(\mathbf{x}_{24})),\ (\mathbf{d}_{41}(\mathbf{s}_{21}(\mathbf{x}_{25}))))\\ &=\mathbf{mod}_4(\mathbf{x}_3,\ \mathbf{x}_{17},\ \mathbf{x}_{24},\ \mathbf{x}_{25})\end{aligned}\tag{23}$$

RESULTS AND DISCUSSION

In the sequential-modular approach the well-known direct or accelerated substitution is used for better convergence. In other numerical methods the evaluation of a flowsheet-level Jacobian is required and we cannot guarantee the convergency and efficiency. The direct substitution method is quite a reliable method compared with other methods. The solution can be expressed as a set of non-linear equations in terms of unknown vector **x** as

$$\mathbf{f}(\mathbf{x})=0 \tag{24}$$

A guess on **x** is made of some stream variables in the loop and calculation of the unit modules produces a new set of values for the guessed stream **g**(**x**). The requirement for a correct guess **x** is

$$\mathbf{x}-\mathbf{g}(\mathbf{x})=0 \tag{25}$$

or

$$\mathbf{x}=\mathbf{g}(\mathbf{x}) \tag{26}$$

The (k+1)th guess for **x** is the value calculated from the kth guess as

$$\mathbf{x}^{k+1}=\mathbf{g}(\mathbf{x}^{k}) \tag{27}$$

This method has an advantage that computation of the inverse matrix can be avoided. The method required many iterations but showed good convergence. Initial guesses can be based on the present operation data. Basic information on tearing streams is given in Table 4. Results of simulations are compared with design data in Table 5, and Table 6 shows a comparison between actual operation data and results of computations. Compositions of each stream can hardly be obtained during operation and only temperature and flowrates are measured. From the comparison we can see little discrepancy between the operation data and computation results. We have to keep in mind that steady-state and equilibrium-stage separation operation are assumed. Even with these assumptions we achieved good agreement between operation and simulation.

CONCLUSION

For the modeling and simulation of the sulfolane extraction process we developed partitioning and tearing techniques based on the reachability matrix and the decomposition algorithm, respectively. For the sulfolane extraction process the algorithm was shown to be simple and easy to use. Due to the solvent regeneration operation the sulfolane extraction process has one strong component that results in serious complexity to compute the whole process. The sequential-modular approach by direct substitution numerical method was applied. Results of computations were compared with actual plant operation data and little discrepancy was found between them.

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NOMENCLATURE

B : any matrix for boolean operation
$\mathbf{d}_{ij}$: module function of jth output of ith divider
$\mathbf{e}_{ij}$: module function of jth output of ith heat exchanger
$\mathbf{f}_{ij}$: module function of jth output of ith separator
$\mathbf{m}_{ij}$: module function of jth output of ith mixer
$\mathbf{mod}_i$: module function based on tearing variables
n : any node in the digraph
N : dimension of any matrix
R : reachability matrix
T(n) : the set of all the immediate successors
$T^{-1}(n)$: the set of all the immediate successors
x : vector of stream
X : arbitrary matrix for example

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