A Numerical Tool for Simultaneous Targeting And Design of Mass Exchange Networks

Wasiu A. Oladosu, Sharifah R.Wan Alwi, Zainuddin A. Manan

Abstract: ***Design of cost-effective Mass Exchange Networks (MENs) that involves mass integration can help to minimize the amount of mass separating agent (MSA) purchased, waste MSA generated by industries, reduce operating costs and mitigate environmental issues associated with MSA disposal. Design of MENs can be done using graphical and numerical methods, as well as using mathematical modelling. This work describes a new approach for simultaneous targeting and design of MENs in which both targeting and network design stage can be solved in a single template, in order to overcome the limitation of graphical tools such as MENs Composite Curves (CCs) and Grid Diagram. CCs cannot completely map individual rich and lean process streams, or process and utility streams. On the other hand, the numerical technique known as Composition Interval Table (CIT) failed to show individual rich and lean stream mass cascades and cannot be used for MENs design. The newly developed numerical approach in this paper employs the Segregated Composition Interval Table (SECIT) to simultaneously locate mass pinch point, determine the minimum utility targets and perform SECIT Mass Allocation (SMA) that can be used to visualize in SECIT Network Diagram (SND).This work can be applied in industries to minimize liquid waste and reduce environmental pollution A case study is presented to demonstrate the validity and advantages of the proposed approach. This paper also shows that SECIT and SND can be a vital combination of numerical and graphical visualization tools for targeting and design of complex MENs.***

Index Terms: Mass exchange networks (MENs), Mass pinch point, Numerical tool, Segregated Composition Interval Table, Minimum utility targets.

I. INTRODUCTION

Utilization of recycle or reuse networks for waste minimization requires the use of mass exchange operations that can transfer hazardous species from a set of rich streams to a set of lean streams. El-Halwagi and Manousiouthakis [1] first introduced pinch analysis to the synthesis of mass exchange network. These authors show how the minimum allowable composition difference**Error! Reference source not found.Error! Reference source not found.** can be used to locate the mass transfer pinch. This ensure a minimum flow rate of external mass-separating agent (MSA) target required by a network to be determined. Several techniques have been proposed to address this problem including mass pinch technology [1], heat and mass exchange networks [2], mathematical programming approaches [3] and batch MEN synthesis [4]. Azeez et al. [5] proposed a new method by exploring key variables such as supply and target composition to define intervals of superstructure. This model is then formulated as mixed interval non-linear program (MINLP) with Total Annual Cost (TAC) minimization as the objective. Recently, Liu et al. [6] introduced a systematic approach for synthesizing combined mass and heat exchange networks. Gadalla [7] developed a graphical method to describe mass exchange network by plotting rich stream composition against equivalent composition for lean stream using pinch analysis principle. However, the performance of the existing MENs was based on the graph obtained. Velázquez-Guevara et al. [8] proposed a general disjunctive programming for optimization and modelling of mass exchange networks that uses state-task-network superstructure. Composition interval table (CIT) is an efficient numerical technique which has been used as an alternative for the Composite curves (CCs) to determine pinch point and the minimum utility requirement because of CIT's advantages in terms of speed and accuracy [1]. A minimum driving force in CIT which is the minimum allowable composition difference ensure a feasible mass transfer from the rich to the lean stream within a given composition interval. The current CIT technique are based on the concept of mass-lumping, which can only determine utility requirement but not for network design. Grid Diagram (GD) are normally used for network design which must be accompanied by repetitive calculations of composition and mass load in order for the placement of mass exchangers across streams. This is because Grid Diagram (GD) is not based on any composition or mass load scale [9]. Wan Alwi and Manan [10] first introduced Streams Temperature versus Enthalpy Plot (STEP) as a graphical tool to map individual profiles of hot and cold streams on temperature versus enthalpy (T-H) diagram to tackle limitations of HEN composite curves. Later Wan Alwi et al. [11] introduced Segregated Problem Table Algorithm (SePTA) for simultaneous targeting and design of heat exchange network. The new SePTA can be used to simultaneously determine the utility target, locate temperature pinch point and perform heat recovery network design. To date, no numerical tool that can be used for simultaneous targeting and design of MENs has yet been reported. The new numerical

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Segregated Composition Interval Table (SECIT) developed can be used to simultaneously the determine the minimum utility targets, composition pinch point and SECIT mass allocation. SECIT Network Diagram (SND) can be used to visualize the amount of mass load transferred and the individual mass exchanger from a rich stream to a lean stream.

II. METHODOLOGY

This section describes the methodology for targeting and design of mass exchange network as shown in Fig.1. The section is divided into three namely: Segregated Composition Interval Table (SECIT), SECIT Mass Allocation (SMA) and SECIT Network Diagram (SND).

A. Segregated Composition Interval Table (SECIT)

This section describes the development of Segregated Composition Interval Table (SECIT) which is an alternative tool to CIT to target the minimum solvent consumption. Tables I and II show rich and lean stream data respectively for case study involving an organic pollutant to be removed from two aqueous stream, rich stream (*R1* and *R2*) and lean streams consisting of two process MSAs (*S1 and S2*) which will be used to illustrate the methodology.

Table I Data of rich streams [12]

Stream	*G(kg/s)*	y_s	y_t	*ΔM(kg/s)*
R1	2	0.030	0.005	0.050
R2	3	0.010	0.001	0.027

Table II Data of lean streams [12]

Stream	L^c*(kg/s)*	x_s	x_t	*G(kg/s)*
S1	17	0.007	0.009	8.5
S2	1	0.005	0.015	2
Stream	y_s	y_t	*ΔM(kg/s)*	
S1	0.016	0.02	0.034	
S2	0.003	0.008	0.010	

Step 1. Data Extraction of Lean and Rich Stream

The rich and lean streams are extracted in terms of G, y_s, y_t for rich stream and L^c, x_s, x_t for lean stream. Next, convert all the lean streams into their corresponding rich value and calculate G for the lean stream as shown in Table II by using (1), (2) and (3) respectively. The minimum allowable composition difference (ε) is 0.001, mass transfer coefficient, m=2 for *S1* and m=0.5 for *S2*; b=0.

$$y_s = m(x_s + \varepsilon) + b \tag{1}$$

$$y_t = m(x_t + \varepsilon) + b \tag{2}$$

$$\Delta M = G(y_s - y_t) \tag{3}$$

Step 2. Determination of Rich and Lean Stream Composition Mass Plot (SCMP)

Arrange the composition of the rich and lean gas streams (y) in decreasing order as shown in Table III, Column 1. Calculate the composition difference (Δy) for each interval and write it in Column 2. Arrange the rich and the lean stream mass flow rate (G) in decreasing order horizontally as shown in (column 3 & 4) for rich and (column 5 & 6) for the lean stream. Arrows can be drawn from each rich and lean stream from supply to target composition. Start by choosing the highest mass flow rate (G) of rich stream in each composition interval to form rich SCMP1 as in (column 7a). In Table III, beginning from the bottom, *R2* is chosen as the first segment of the rich SCMP1 because only *R2* exist between composition interval of 0.001 and 0.003. Also, *R2* exist between 0.003 and 0.005, hence *R2* is chosen. Between 0.005 and 0.008, both *R1* (G=2) and *R2* (G=3) exist. *R2* is chosen because *R2* has a larger mass flow rate than *R1*. Between the interval 0.01 and 0.016 only *R1* exist, hence *R1* is chosen.

The next continuous rich SCMP is constructed by extracting the next highest mass flowrate rich stream with multiple streams from the intervals. For instance, Rich SCMP2 (column7b) is constructed from the remaining rich stream after Rich SCMP1 is completed. Only stream *R1* exist between composition intervals 0.005 and 0.008, and hence *R1* is chosen. The same procedure occurs for composition interval 0.008 and 0.01, *R1* is also chosen to form SCMP 2. Next, construct the continuous lean SCMP (column 7c). For example, lean SCMP1 in Table III shows that between 0.003 and 0.005 only *S2* exist, Hence *S2* is chosen in the interval. The same procedure applies for streams in the two remaining composition intervals as shown in column 7c. Table III shows the final continuous rich and lean SCMP. There are two rich SCMPs namely Rich SCMP1 (column 7a) and Rich SCMP2 (column 7b) and only one lean SCMP, namely lean SCMP1 (column7c).

Step 3. Determine the net mass flow rate for composition intervals

The net mass flow rate, **Error! Reference source not found.**between each rich and lean SCMP are determined by (4). See Table IV of column 3a and 3b. The net G for SCMP1 in Table IV of column 3a is derived by subtracting the mass flow rate (G) for Rich SCMP1 (column 7a) in Table III from the mass flow rate G of Lean SCMP1 (column 7c) in Table III. Repeat the same procedure for SCMP2 in column 3b of Table IV.

$$G_{net} = G_R - G_L \tag{4}$$

Step 4. Determine net mass requirement for each composition intervals

The net mass requirement is obtained by multiplying the net mass flow rate for each SCMP and the composition interval to obtain net mass surplus or deficit for a given interval (see Table IV in Columns 4a and 4b).

Step 5. Calculate the cumulative mass cascade

Cascading is done from higher concentration to lower concentration in MENs because component is usually transferred from rich streams to lean streams. The cumulative mass cascade is

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calculated by using (5). The cumulative mass across a given composition interval, ΔM is obtained by adding the mass cascade at a higher composition interval **Error! Reference source not found.** (**Error! Reference source not found.** and the net mass change at the interval *i***Error! Reference source not found.**See Table IV of Columns 5a and 5b.

Fig.1 Algorithm diagram for simultaneous targeting and network design using SECIT

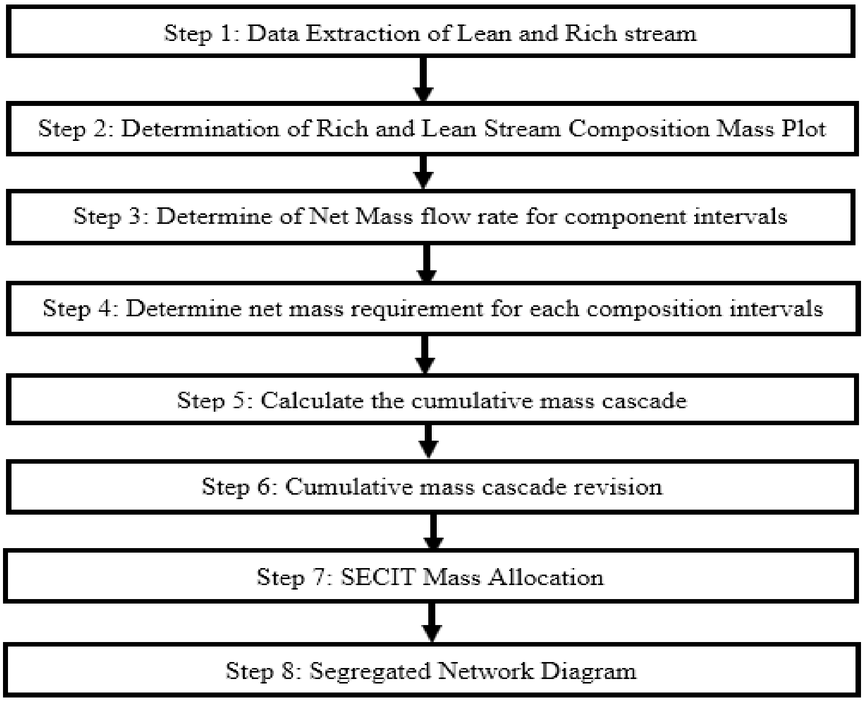

Table III Determination of Rich and Lean SCMP

	1	2	3	4	5	6	7a	7b	7c
j	*y*	*Δy*	***R2***	***R1***	***S1***	***S2***	**Rich SCMP1**	**Rich SCMP2**	**Lean SCMP1**
		G	**3**	**2**	**8.5**	**2**			
1	0.03								
		0.01					*R1*		
2	0.02								
		0.004					*R1*		*S1*
3	0.016								
		0.006					*R1*		
4	0.01								
		0.002					*R2*	*R1*	
5	0.008								
		0.003					*R2*	*R1*	*S2*
6	0.005								
		0.002					*R2*		*S2*
7	0.003								
		0.002					*R2*		
8	0.001								

Table IV Utility targeting for Single Pinch Problem

1	2	3a	3b	4a	4b	5a	5b	6a	6b
y	**Δy**	**Net mass flow rate (G_R-G_L)**		**Δ*M***		**Cumulative Mass (Δ*M*)**		**Feasible Cumulative Mass (Δ*M*)**	
		SCMP1	**SCMP2**	**SCMP1**	**SCMP2**	**SCMP1**	**SCMP2**	**SCMP1**	**SCMP2**
0.03						0		0.006	0
	0.01	2		0.02	0				
0.02						0.02	0	0.026	0
	0.004	-6.5		-0.026	0				
0.016						-0.006	0	0	0
	0.006	2		0.012	0				
0.01						0.006	0	0.012	0
	0.002	3	2	0.006	0.004				
0.008						0.012	0.004	0.018	
	0.003	1	2	0.003	0.006				
0.005						0.015	0.01	0.021	0.004
	0.002	1		0.002					
0.003						0.017		0.023	0.01
	0.002	3		0.006					
0.001						0.023		0.029	

$$\Delta M_{cas,i} = \Delta M_{cas,i-1} + \Delta M_{\text{int},i} \quad (5)$$

Step 6. Cumulative mass cascade revision

Mass cascade table in Step 5 may contain negative mass flows. To obtain a feasible mass cascade such as those shown in (Column 6a and 6b) of Table IV, the absolute value of the largest negative from the cumulative mass cascade (Column 5a and Column 5b) of Table IV is added to the top of the feasible mass cascade column (Column 6a and 6b) and cascaded down the composition interval to yield the minimum utility requirement. If there is no negative value, it means the original zero value is maintained as the initial cascade. The Segregated Composition Interval Table (SECIT) result shows that the fresh MSA target is 0.039kg/s and 0.006kg/s of waste solvent. The global pinch point is 0.016 which is the composition interval where both SCMP 1 and SCMP2 have zero values in the feasible mass cascade columns.

B. SECIT Mass Allocation (SMA)

The results from SECIT can be extended to illustrate how mass is being allocated in the mass exchange network. The SECIT mass allocation procedure from the rich stream to the lean stream is described below:

a) The selected rich and lean SCMP with the corresponding mass flow at each composition intervals are listed as shown in Table V of Columns 3b, 3e, 4b and 4e.
b) Cascade the available mass beginning at top of the column from rich SCMPi to lean SCMPi down the interval composition as in Columns 3c and 4c.
c) To achieve minimum utility target, no mass is transfer across the pinch. Complete SECIT mass allocation between individual rich and lean streams are shown in Table V.

C. Segregated Network Diagram (SND)

The SMA can be easily visualized by using a network diagram that represents the rich and lean streams, and the connecting mass exchangers. The SECIT network diagram shows the mass exchange allocation according to the supply and target composition as well as the corresponding mass load. The completed SECIT mass allocation is transformed to the overall SND shown in Fig.2. A total of 0.01kg/s and 0.029kg/s of external mass separating agent (MSA), are needed for *R1* and *R2*. The External Mass Utility EMU 1, (0.012kg/s) depicted in a rectangular box is the utility to reduce the organic pollutant composition in stream *R1* from 0.011 to 0.005. Also, EMU 2, (0.027kg/s) is needed to reduce the organic pollutant composition in stream *R2* from 0.01 to 0.001. The first mass exchanger, ME1(0.028kg/s) exchange mass between stream *R1* from 0.03 to 0.016 with *S1* from 0.016 to 0.019 leaving an excess MSA of 0.006kg/s.

Stream *R1* from composition of 0.016 to 0.011 is matched with *S2* from 0.003 to 0.008 via ME 2 with mass load of 0.01kg/s.

Table V SECIT Mass Allocation (SMA)

1	2	3a	3b	3c	3d	3e	4a	4b	4c	4d	4e
		SCMP 1					SCMP 2				
y	Δy	Rich stream	Rich SCMP1 ΔM	Stream Match	Lean Stream	Lean SCMP1 ΔM	Rich stream	Rich SCMP2 ΔM	Stream Match	Lean Stream	Lean SCMP2 ΔM
0.03		ExcessMSA	0.006								
	0.01	*R1*	0.02	0.006 0.02							
0.02											
	0.004	*R1*	0.008	0.008	*S1*	0.034	ExcessMSA	0			
0.016				PINCH	POINT						
	0.006	*R1*	0.012								
0.01				0.006							
	0.002	*R2*	0.006				*R1*	0.004			
0.008				0.004					0.004		
	0.003	*R2*	0.009	0.006 0.002	*S2*	0.006	*R1*	0.006	0.006	Ext.MSA	0.01
0.005				0.009							
	0.002	*R2*	0.006		*S2*	0.004					
0.003				0.006							
	0.002	*R2*	0.006	0.006							
0.001					Ext.MSA	0.029					

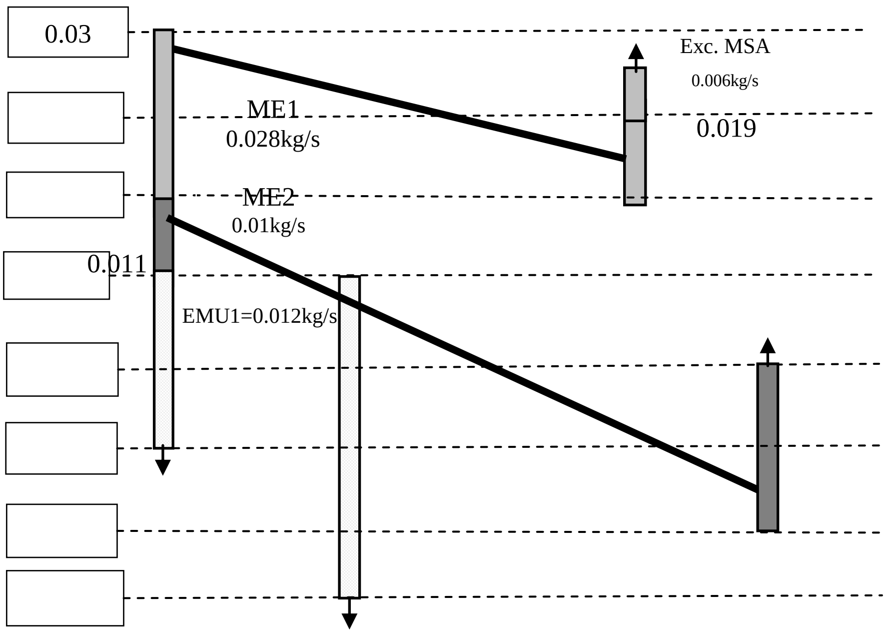

Fig. 2 SECIT Network Diagram (SND)

III. RESULTS AND DISCUSSION

Mass cascade that gives global pinch point composition and the minimum utility requirement are shown in Table IV. The excess Mass Separating Agent (MSA) is MSA=0.006 kg/s for SCMP1 and Excess MSA =0 kg/s for SCMP 2 which is the mass added in column 6 of Table IV. On the other hand, the External MSA is the cumulative mass in the final composition in column 6 of Table IV. For example, External MSA=0.029 kg/s for SCMP1 and External MSA=0.01 kg/s for SCMP2. The pinch composition was obtained at feasible mass cascade interval where the net mass flow is zero. From Table IV, the Excess MSA is the sum of the mass for the two SCMP, which is equal to 0.006 kg/s and the External MSA needed to remove the organic pollutant is the sum of the two SCMP, i.e. (0.029+0.01) = 0.039 kg/s. The global pinch composition for this problem is 0.016 .The results are summarized in tabular form as shown in Table VI. The results obtained agrees with the results reported using other methods such as CC and CIT [12].

Table VI: Result Summary

Mass Separating Agent (MSA)	Stream Composition Mass Plot (SCMP 1)	Stream Composition Mass Plot (SCMP 2)
Excess MSA (kg/s)	0.006	0.00
External MSA (kg/s)	0.029	0.01
Global Pinch Point	0.016	

IV. CONCLUSION

A new numerical tool has been introduced for simultaneous targeting and design of mass exchange network. The Segregated Composition Interval Table (SECIT) are profiles of mass cascade based on composition interval for the rich and lean stream. The SECIT can simultaneously show the pinch point, minimum external mass separating agent and SECIT mass allocation. The SECIT mass allocation can also be represented on the SECIT network diagram to show the mass exchange network. SECIT can become an alternative visualization tool for simultaneous targeting and design of Maximum Mass Recovery (MMR) Networks which can overcome the limitations of composition interval table and grid diagrams.

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