

New Hybrid Method for Mass Exchange Network Optimisation

Abdulfatah M. Emhamed^a, Zoltan Lelkes^{a*}, Endre Rev^a, Tivadar Farkas^a, Zsolt Fonyo^a
and Duncan M. Fraser^b

^aBudapest Univ. of Technology and Economics, Department of Chemical Engineering
H-1521, Budapest, Hungary

^bUniversity of Cape Town, Department of Chemical Engineering
Private Bag, Rondebosh, 7701, South Africa

Abstract

A new hybrid optimisation method is presented, that is fairly robust and can be accomplished in an automatic way. The main idea is using integer cuts and bounds, calculated based on driving force plot analysis, for the lean streams to decrease the possibility of being trapped in local optimum. A new initial solution is constructed only if the MINLP solution is infeasible, otherwise the best solution found earlier is used. In consequence, the MINLP model changes in the iteration steps. The iteration is stopped if the total annual cost (TAC) in the solution is less than $1.1 \cdot TAC_{\text{target}}$.

Keywords: Mass Exchange Networks, Optimisation, Pinch Technology

1. Introduction

The mass exchange networks (MENs) are systems of interconnected direct-contact mass-transfer units using process lean streams or external mass separating agents (MSAs) to selectively remove certain components (often: pollutants) from rich process streams. The process is depicted in Figure 1.

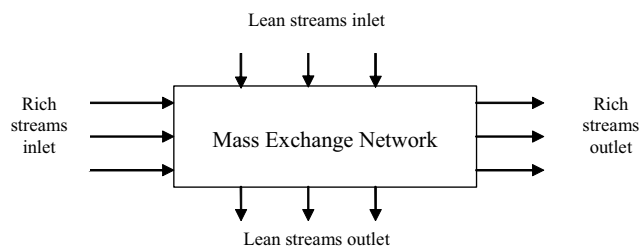


Figure 1. Mass Exchange Network

The notion of mass exchange network synthesis (MENS) and a pinch based solution methodology were first presented by El-Halwagi and Manousiouthakis (1989).

* Author to whom correspondence should be addressed: lelkes@mail.bme.hu

Subsequently, Papalexandri et al. (1994) presented a mixed integer non-linear programming (MINLP) design technique for MENS. Later, Hallale and Fraser (1998) extended the pinch design method by setting up capital cost targets ahead of any design. Recently, Comeaux (2000) and Sztikai et al. (2003) presented optimisation based design methodologies, where pinch insight is applied to develop a superstructure which is, in a later step, optimised by MINLP. The idea of hybrid synthesis method of mass exchange network was first presented by Msiza and Fraser (2003).

One of the main difficulties in optimising MENS by MINLP is the non-linearity of the model equation system. Even using a fairly linear model, based on pinch insight superstructure (Sztikai et al., 2003), the component balance around units remains non-linear. Another difficulty is structural multiplicity (i.e. different solutions can represent the same flowsheet) in all the hitherto known superstructures formulated for MENS. Global optimum is not guaranteed, and the results strongly depend on initial values. That is why we have developed a systematic methodology for solving this problem.

The main drawbacks of the first hybrid synthesis method elaborated by Msiza and Fraser(2003) are (1) the need for assignment of new initial structure, which is a very time consuming step, and (2) the need for human interactivity in the algorithm.

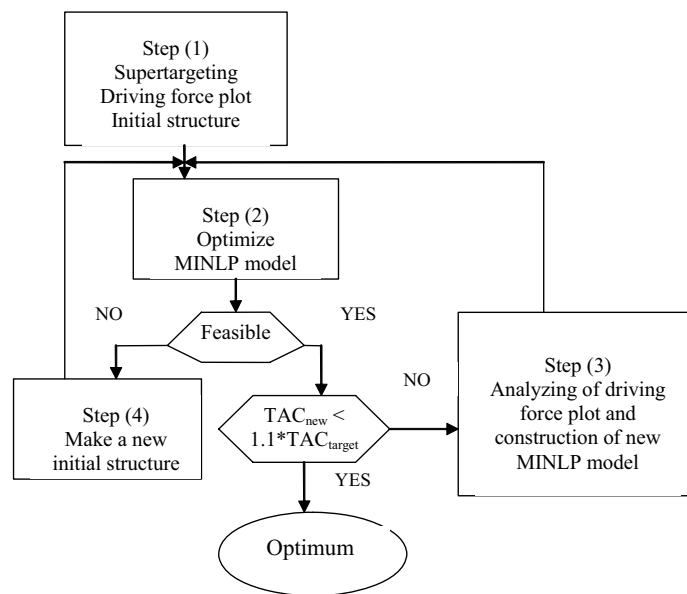


Figure 2. Algorithm of new hybrid method

2. General algorithm of the new hybrid method

The main idea of our new hybrid method is using integer cuts and bounds to the lean streams in order to exclude the local optimum found earlier. The MINLP model developed by Sztikai et al. (2003) is applied because its superstructure is based on pinch insight and, therefore, this model is more suitable for a hybrid method than that of Papalexandri et al. (1994).

The scheme of the new hybrid method algorithm is shown in Figure 2. Supertargeting with the method of Hallale and Fraser (1998) is performed first, determining TAC (total annual cost) target TAC_{target} . 110 % of its value is used as a stop criterion in the iterative process. Driving force plot (DFP) to the minimum external lean stream flow rates is drawn and, then, an initial flowsheet is determined. An MINLP technique is used in the second step to optimise the flowsheet. If the TAC in the solution reaches $1.1 * TAC_{target}$ from above, then the iteration is stopped. Otherwise, the MINLP model is complemented with an integer cut to exclude the local optimum found, and with flow rate bounds calculated on the base of DFP analysis. Initial solution is constructed only if the MINLP solution is infeasible; otherwise, the best feasible solution found till that point is used. Thus, the MINLP model changes in the iteration steps. The steps of the new hybrid method are detailed and illustrated in the next section on the task of optimising a middle scale MENS problem.

3. Demonstration of the new hybrid method

3.1 Problem statement

Remove ammonia from five gas streams, mainly from air (example 4.1 in Hallale's Thesis, 1998). Three water-based streams are available for service. Two of them are processes MSAs, S1 and S2, and one is an external MSA, S3. Stream data are given in Table 1. Carbon steel packed columns, packed with 25.4 mm Raschig rings, are used as mass exchangers, with $K_{\mu}=0.02$ kg NH_3 /s/kg exchanger mass lumped coefficient, and shell cost $\$618M^{0.66}$, where M is exchanger mass (kg). Cost of S3 is 0.001 \$/kg.

Table 1. Stream data for example problem

Rich Streams	G (kg/s)	y^s (mass fraction)	y^t (mass fraction)		
R1	2	0.005	0.0010		
R2	4	0.005	0.0025		
R3	3.5	0.011	0.0025		
R4	1.5	0.010	0.0050		
R5	0.5	0.008	0.0025		
MSAs	L^c (kg/s)	x^s (mass fraction)	x^t (mass fraction)	m	b
S1	1.8	0.0017	0.0071	1.2	0
S2	1	0.0025	0.0085	1	0
S3	∞	0	0.017	0.5	0

3.2 The steps of the new method

3.2.1 Step 1:

Step 1 includes three parts to complete the preparation of the hybrid method. First the supertarget for the problem is determined by pinch technique, then the initial flowsheet is developed and the driving force diagram is plotted. Using the pinch technique developed by Hallale (1998), the TAC target for this problem is determined. The total annual cost target (TAC_{target}) is 788,405 \$/yr at 0.0007 minimum approach composition. The simplest way of constructing an initial structure is using only one of the external

streams in a parallel structure. In our case the only external stream is the S3; thus, the mass flow rate of S3 needed to remove the ammonia from the five rich streams is computed. The initial structure worked out for this problem is shown in Figure 3. The method of constructing a DFP is discussed in detail by Hallale (1998). The composite operating line calculated for the minimum external flowrate and the exchangers' driving forces of the initial structure are plotted in Figure 4. The driving forces of exchangers 3, 4, and 5 are too high compared to the composite operating line, indicating that the initial flowsheet is far from the optimum.

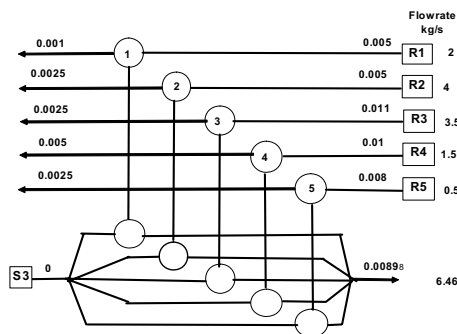


Figure 3. Initial structure of the problem

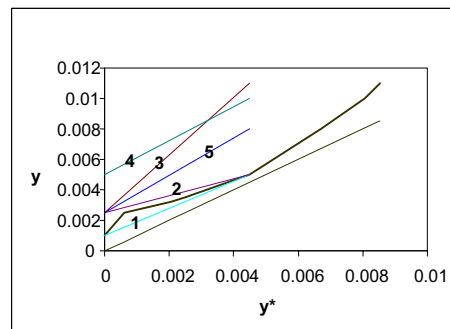


Figure 4. Driving force plot and driving forces of the initial structure

3.2.2 Step 2

MINLP optimisation is accomplished. The MINLP model is implemented in GAMS (Brook et al, 1998) and solved using the Outer Approximation algorithm (with the solver DICOPT) on a SUN Sparc Station. If a feasible solution is found (TAC_{new}), the criterion $TAC_{new} \leq 1.1 * TAC_{target}$ is checked. The iteration is stopped if the optimum TAC_{new} found is better than 110 % of TAC_{target} , otherwise Step 3 is executed. In the case of an infeasible MINLP solution, a new initial structure is constructed in Step 4. $TAC = 928,342$ \$/yr was found by MINLP optimisation in the first iteration; the structure and the driving force of this result are shown in Figures 5 and 6. Although the new solution is better than the initial one according to the comparison of the driving force plots (Figures 4 and 6), the new TAC does not reach the stop criterion. Therefore, a new MINLP model is to be constructed, based on DFP analysis, in Step 3.

3.2.3 Step 3

A new MINLP model is constructed excluding the former binary solutions by using integer cuts, and by using the best local solution, hitherto found, as the new initial structure. An upper or lower bound to a lean stream flow rate is inserted to the MINLP model, based on DFP analysis. An upper bound is used if the driving forces of the units are on the average higher than the composite operating line, otherwise a lower bound is used. The new bound must be tighter than what was used in the last MINLP model, and must be defined for the stream belonging to the least efficient unit.

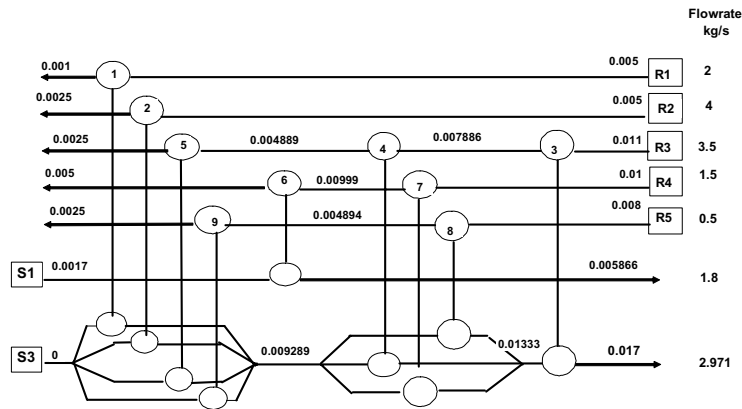


Figure 5. MINLP solution of iteration 1

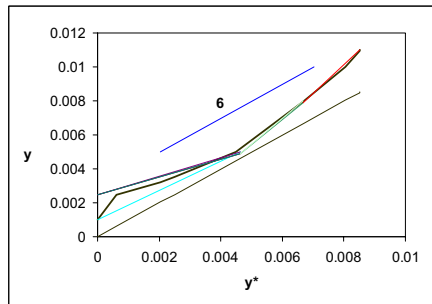


Figure 6. Driving force plot based on the MINLP solution of iteration 1

If the least efficient unit cannot be unambiguously selected then the streams of the candidate units are compared by the following efficiency factors. For upper bound: $E_j^{UP}=A/M$; for lower bound: $E_j^{LO}=(B-A)/M$; where A is the actual mass exchange of stream j ; B is the total mass exchange that can be performed by using stream j ; and M is the total mass exchange of the whole system. Based on E_j^{UP} and E_j^{LO} , the stream having the highest efficiency is selected, and the upper or lower bound is defined for it.

The least efficient unit can easily be selected by analyzing the DFP of the flowsheet found in the first iteration (see Figure 6). The least efficient unit is unit 6; and its lean stream is S1. The first solution had been excluded by an integer cut, and a new upper bound for stream S1 had been introduced, but then MINLP optimisation led to an infeasible solution; therefore, a new initial structure was subsequently constructed in this iteration step, as is described below in *Step 4*.

3.2.4 Step 4

A new initial structure is generated here. In order to exclude the human factor as much as possible, constructing a new initial structure is based on the efficiencies of lean streams. The flowrate of the least efficient stream is changed in order to increase its efficiency. This can give rise to the need for creating a new unit, or for changing the streams of the existing units.

After constructing a new initial structure, the MINLP optimisation (in *Step 2*) found a new feasible solution with TAC=894,872 \$/yr.

3.3 Final solution

The optimal solution of the problem has been found in 5 iteration steps. The improvement of the TAC is shown in Table 3. The TAC of the optimal structure is 808,986 \$/yr. The structure of the optimal solution is shown in Figure 7.

Table 3. MINLP results in subsequent iterations

N° of iteration:	1	2	3	4	5
TAC (\$/year):	928,342	infeasible	894,872	868,571	808,986

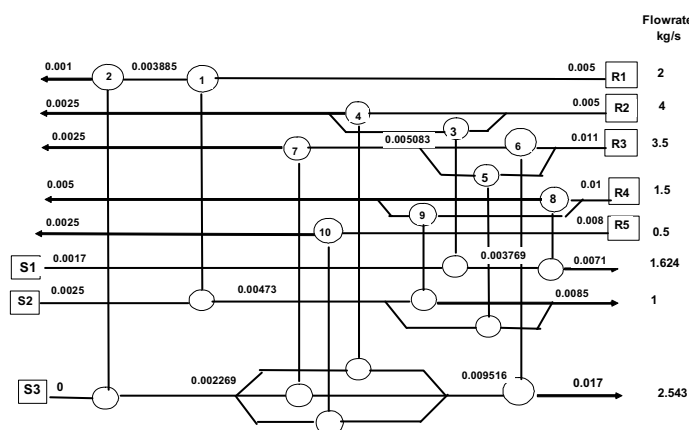


Figure 7. Final structure

4. Conclusion

A new hybrid optimisation method for MENS is developed. The new method uses integer cuts and bounds, calculated on the base of DFP analysis, in the MINLP formulation. A new initial solution is constructed only if the MINLP problem is infeasible. The method has been demonstrated on a middle scale MENS problem involving five rich and two process lean stream, and one external lean stream. The optimal solution has been found in five iteration steps, by successive improvements. The new method is fairly robust and can be accomplished in an automatic way.

References

- Brooke, A., D. Kendrick, A. Meeraus and R. Raman, 1998, GAMS, A user's guide. GAMS Development Corporation, Washington.
- Comeaux, 2000, MSc. Thesis. UMIST.
- El-Halwagi, M. M. and V. Manousiouthakis, 1989, AIChE Journal, 35(8), 1233.
- Hallale, N. and D. M. Fraser, 1998, Chem. Eng. Sci. 53(2), 293.
- Hallale, N., 1998, PhD Thesis. University of Cape Town.
- Msiza A. K. and D.M. Fraser, 2003, Computer-Aided Chemical Engineering 14. Elsevier, 227.
- Papalexandri, K. P., E.N. Pistikopoulos and C.A. Floudas, 1994, Trans. Inst. Chem. Eng. 72, 279.
- Szitkai, Z., T. Farkas, Z. Kravanja, Z. Lelkes, E. Rev and Z. Fonyo, 2003, Computer-Aided Chemical Engineering 14. Elsevier, 323.

Acknowledgements

This study was partially supported by OTKA T037191 and OTKA F046282.