DESIGN AND SYNTHESIS OF DISTILLATION SYSTEMS USING A DRIVING FORCE BASED APPROACH

Erik Bek-Pedersen and **Rafiqul Gani**

CAPEC, Department of Chemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

ABSTRACT

A new integrated framework for synthesis, design and operation of distillation based separation schemes is presented here. This framework is based on the driving force approach, which takes advantage of differences in chemical/physical properties between two co-existing phases in a separation unit.
A set of algorithms has been developed within this framework for design of simple and complex distillation columns, for sequencing of distillation columns, determination of operating conditions and for generating hybrid separation schemes as well as retrofit of distillation columns. The main feature of all these algorithms is that they provide a "visual" solution that also appears to be near optimal in terms of energy consumption. Several illustrative examples highlighting the application of the integrated approach are also presented.

Keywords: Driving force, distillation, integrated system, synthesis, design, optimal solution

INTRODUCTION

Separation processes usually make use of some kind of driving force to achieve the desired separation. Therefore it is advantageous to perform a driving force analysis at the earliest possible stage of the design of a process. Driving forces exploit differences in chemical/physical properties between two co-existing phases in a separation unit. So, if the feed mixture, which has to be separated, is a homogeneous single phase solution, the generation or addition of a second phase is essential to perform a separation. The driving forces can be generated or caused by various techniques related to different chemical/physical properties. In distillation and evaporation the driving force is the difference in composition between the vapor phase and the liquid phase, which is caused by a difference of properties such as boiling point and vapor pressures. As the driving force approaches zero, separation of the corresponding key component from the mixture becomes difficult while as the driving force approaches a maximum, the energy necessary to maintain the two-phase system is a minimum. This is because the driving force is inversely proportional to the energy added to the system to create and maintain the two-phase (vapour-liquid) system. Therefore, distillation design based on maximizing the driving force may lead to a highly energy efficient design.

The methodology presented here consists of calculation of the driving force for the pair of key (binary pair) components of a binary or multi-component mixture, plotting of the driving force as a function of composition, identifying the location of the maximum driving force and based on this, determining the design such as feed location, reflux ratio, reboil ratio and number of plates together with estimates of the column composition and temperature profiles. Adding the bubble point pressure curve to the driving force diagram gives the column pressure [2]. One advantage of this method is that the driving force based design is visual (graphic) and does not need any rigorous calculations. Yet, the driving force based methodology provides a near optimal design with respect to energy consumption. It also provides a physically feasible distillation design.

In this paper, the driving force based design will be presented and highlighted through several separation by distillation problems. Distillation column design for simple columns (one feed with two products), for complex columns (one or more feed and/or side products), for separation of binary as well as ternary and/or multi-component mixtures and for distillation column sequencing (multi-component separations). These visual techniques are valid for equilibrium as well as non-equilibrium systems and ideal as well as non-ideal and/or reactive systems. The visual tools based design is validated through rigorous simulation. It will be shown that the rigorous solution not only lies close to the optimal solution but that the results from the visual design provides such a good initial estimate that convergence in the steady state solution is always achieved.

METHOLOGY

The driving force as defined by Gani and Bek-Pedersen [3] is given by,

$$F_{ij} = y_i - x_i = \frac{x_i \beta_{ij}}{1 + x_i(\beta_{ij} - 1)} - x_i \qquad (1)$$

In the above equation, x_i and y_i are the compositions of component i in two co-existing phases, F_{ij} is the driving force for component i, β_{ij} is the relative separability factor for component i with respect to property (or separation technique) j. Note that β_{ij} = f(T, P, composition, θ), where θ indicates external factors such as resistance to mass transfer and heat transfer. From Eq. 1, it can also be noted that at fixed P (or T), two-dimensional plots of $|F_{ij}|$ versus x_i (or y_i) can be made where each data point may also indicate a different T (or P). Therefore, these diagrams can be used to design and configure separation schemes, including conditions of operation.

Gani and Bek-Pedersen [3] have already shown how the driving force diagrams with respect to relative volatility can be used for near optimal (with respect to energy consumption) single distillation column design. Bek-Pedersen et al. [1] have shown how the driving force diagrams can be used to obtain near optimal (with respect to energy consumption) sequence of distillation trains. Bek-Pedersen et al. [2] extended and modified these algorithms to allow for the presence of azeotropes in the multi-component mixtures, to generate hybrid separation schemes and to allow for scaling in the distillation column design when "extreme" conditions for the feed mixture or product compositions are specified. Note that, as the location of the feed point on the D_x-D_y line is determined (see Figure 1), the corresponding reflux and reboil ratios are also determined, based upon knowledge of the products, A and B. For only one high purity product, it is necessary to relocate the feed point in order to achieve the optimal combination of reboil and reflux ratios. Effects of non-key components are taken into account through mixture analysis related to mutual solubility, azeotropic data and dependence of the separation factor on the composition.

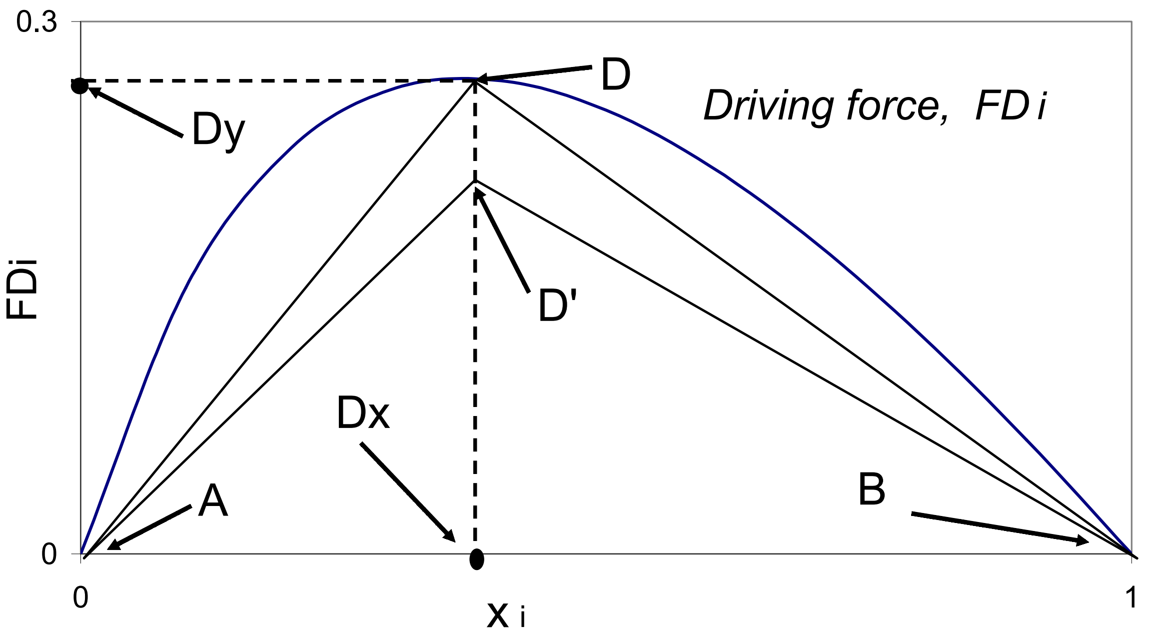


Figure 1: Driving force diagram for constant β_{ij} = 3.

Six algorithms related to separation synthesis and retrofit design have been developed. The first algorithm deals with the single column distillation and forms the basis of the whole work, and therefore also the other algorithms. The second algorithm is for the design of complex distillation columns. The third algorithm deals with the sequencing of simple distillation columns for multi-component separations and the corresponding conditions of operation. The fourth algorithm deals with generation of hybrid separation schemes. The fifth algorithm is for pressure allocation in a sequence of distillation columns. The last algorithm deals with retrofit design of distillation columns. This algorithm requires that the number of plates and the (potential) feed plate location(s) are known. Algorithms 1 and 2 are illustrated through Figure 1, where it is illustrated how the easiest separation is obtained by applying the largest driving force. In this paper all previously developed algorithms and new design algorithms have been integrated in a single framework for synthesis and design of distillation based separation systems. First we will go through the algorithms individually.

Algorithm 1: Single distillation column design.

1. Generate or retrieve from a database, the vapor-liquid data for the binary system in the column. For a multi-component system, select the two key components to define the "split" and use them as the binary (key) mixture.

2. Calculate the driving force between the two (key) components at the actual operating pressure. Plot the calculated driving force as a function of the light key component.

3. Locate the point Dx as the point on the x-axis that corresponds to the largest driving force.
   3.1. In case of an azeotrope, re-scale the x-axis and locate the point Dx as the relative distance between the two points, one on each side of D, where the driving force is zero on the x-axis. (The two points are the azeotropic point and the bottom/top product).

4. Calculate the minimum reflux ratio.

5. Give the desired product specifications.

6. Determine whether rescaling needs to be applied. If condition 1 or 2 is satisfied, scaling is needed. Go to 7, otherwise go to 8.

7. If condition 1 is satisfied, go to 7.1. Else condition 2 is satisfied and go to 7.2.
   7.1. If condition 1a is satisfied, then relocate N_F between 5 % and 10 % up in the column.
   Else condition 1b is satisfied, then relocate N_F between 5 % and 10 % down in the column.
   7.2. If condition 2a is satisfied, then relocate N_F 10 % down.
   Else, if condition 2b is satisfied, then relocate N_F 5 % down.
   Else, if condition 2c is satisfied, then relocate N_F 5 % up.
   Else, if condition 2d is satisfied, then relocate N_F 10 % up.

8. Apply equation 1 (taking the scaling factors determined in step 4 into consideration) to compute N_F for a given value of N.

$$N_F = N \cdot (1 - D_X) \tag{2}$$

Condition 1:

a) $x_{HK,Z} > 0.8$ and $Dx < 0.7$

b) $x_{LK,Z} > 0.8$ and $Dx > 0.3$

Condition 2:

a) $\frac{1-x_{LK,D}}{1-x_{HK,B}} < 0.01$ and $Dx < 0.7$

b) $\frac{1-x_{LK,D}}{1-x_{HK,B}} < 0.1$ and $Dx < 0.7$

c) $\frac{1-x_{HK,B}}{1-x_{LK,D}} < 0.1$ and $Dx > 0.3$

d) $\frac{1-x_{HK,B}}{1-x_{LK,D}} < 0.01$ and $Dx > 0.3$

Z, B, D refer to feed, bottom and distillate respectively. HK and LK are heavy and light key components.

Algorithm 2: Design of complex distillation columns (1 feed and 3 products).

1. List the 3 key compounds according to their boiling points.
   No. 1 is the lightest boiling,
   No. 2 is the intermediate boiling,
   No. 3 is the heaviest boiling.

2. Generate or retrieve VLE data for component 1 and 2, and for component 2 and 3.

3. Check if No. 1 and No. 2, or No. 2 and No. 3 form an azeotope. If yes: Stop.

4. Calculate and plot the 2 driving force diagrams corresponding to the 2 sets of VLE data.

5. Determine which of the 2 plots exhibits the larger driving force.

6. Configure the column accordingly.
   6.1. If the largest driving force occurs between components no. 1 and 2, then the feed should be between the top and the side-draw in the column.
   6.2. Else, if the largest driving force occurs between components no. 2 and 3, then the feed should be between the bottom and the side-draw in the column.

7. Generate the joint driving force curve such that the largest total driving force is achieved.
   7.1. If the feed is introduced between the top and the side draw, then the driving force curves should be joined such that the largest driving force is in the top of the column.

7.2. Else, if the feed is introduced between the bottom and the side draw, then the driving force curves should be joined such that the largest driving force is in the bottom of the column.

8. Give the number of plates, N, in the column.

9. Calculate the minimum reflux required in the column.

10. Give specifications on the products. Note that the size of the side-draw must be consistent with the overall mass balance of the column.

11. From the joint driving force curve, determine the near optimum position of the side draw stage.
    11.1. Locate the point Ds, where the two driving force curves intersect.
    11.2. Calculate the near optimum position of the side draw stage from $N_S = N(1-D_S)$, where N is counted from the top.

12. From the binary driving force plot that exhibits the largest driving force, locate the near optimum feed stage location.
    12.1. Locate the point D_X, the position on the composition axis corresponding to the largest driving force.
    12.2. If the feed is introduced above the side draw, then calculate the near optimum feed stage from $N_F = N_S(1-D_X)$, where N_S is counted from the top. (Note N_S is used instead of N because there are only N_S stages in the sections represented by the driving force plot.)
    12.3. Else, if the feed is introduced below the side draw, then calculate the near optimum feed stage from $N_F = N_S+(N-N_S)(1-D_X)$.

<u>Algorithm 3: Sequencing of distillation columns.</u>

1. Retrieve the vapour-liquid data available for each pair of adjacent key components.

2. List all the components in the mixture, NC, according to their relative separability factor, β_{ij}.

3. Calculate the driving force diagrams for the adjacent components, at a specified pressure. In total, driving force diagrams for NC-1 binary pairs are calculated. Set k = 1.
    3.1. If a binary pair forms an azeotrope, multiply the maximum driving force by a penalty weight $\left(\left(\frac{D_{y,min}}{D_{y,max}}\right)\cdot D_{y,azeotrope}\right)$ to make the value the smallest among the binary pairs.

4. For split k, select the adjacent pair for which the maximum driving force has the largest value.

5. Remove split k from the list of binary pairs. Set k = k+1 and repeat the algorithm from step 4 until only one split remains to be allocated.

6. Draw the flowsheet based on the selected order of the splits.

7. If allocation of column operating pressures is desired go to algorithm 5. Otherwise go to step 8.

8. For each column, perform the distillation column design through algorithm 1.

Note that this sequencing algorithm provides the largest total driving force for the generated flowsheet. In this way the overall separation becomes the easiest possible, and will thus require the least amount of energy input.

Algorithm 4: Generation of hybrid separation sequence.

1. For a binary pair that forms an azeotrope (or eutectic points or exhibits mutual solubility), retrieve all sets of two-phase composition data, where each set corresponds to a different separation technique. Note: two sets of data at different operating conditions for the same separation technique are considered here as different separation techniques.

2. Calculate and plot all the corresponding driving force diagrams.

3. For the specified product purities, identify all feasible paths, allowing a switch from one separation technique to another if necessary, by moving along the driving force curves (see Figure 4a). Note: if one separation technique is unable to achieve the desired separation, switch to another that is feasible.

4. For each feasible path, identify the corresponding separation techniques and operating conditions from the driving force diagram.

5. Select as the initial flowsheet, the one with the largest total driving force.

6. Use the information from steps 4 and 5 to formulate and solve a structural optimisation problem to determine the optimal flowsheet.

This algorithm gives an optimisation problem as result, and can thus not itself give an optimal solution. Different types of processes and their associated cost factors may need to be considered.

Algorithm 5: Operating conditions.

1. Calculate data for the p-x-y diagram for the two key components in the first distillation column at the bubble point temperature of the feed. Set k=1.

2. Draw the driving force curve from the data calculated in step 1 together with the bubble point curve.
   2.1. Identify the point D_x as the composition x_i, where the driving force reaches its maximum value (D_y).

2.2. Identify the bubble point pressure at the point D_x. Allocate this pressure as the operating pressure for the condenser in distillation column k.
2.3. Based on a specified pressure drop per plate, determine the reboiler pressure for column k.

3. Calculate p-x-y diagrams for the two key components in the next distillation column (k+1) as a function of the temperature. Identify the temperature at which the p-x-y diagram gives the maximum bubble point pressure to within 5 % of the reboiler pressure of column k. Select this temperature as the feed temperature.

4. Repeat step 3 until all the condenser and reboiler pressures have been allocated in the distillation column sequence.

Note: If the pressure in one or more of the columns in the distillation train is found to be lower than atmospheric, a higher pressure in the first column should be considered as an alternative.

<u>Algorithm R1: Retrofit design of distillation columns.</u>

1. Determine the desired products.

2. Find out the FDi_{Max} of the column from Table 1 (use linear interpolation, if necessary).

3. Find the corresponding range of relative volatilities, α, that will correspond to this FDi_{Max} from Figure 2.

4. Find the minimum reflux ratio RR_{min} and actual reflux ratio RR.

5. Check if the mixture exhibits this range of α. If yes, go to 7, otherwise go to 6.

6. Search a database or other knowledge bases to identify solvent candidates that also match the target α on a solvent-free basis.

7. Apply algorithm 1 to verify the feed location.

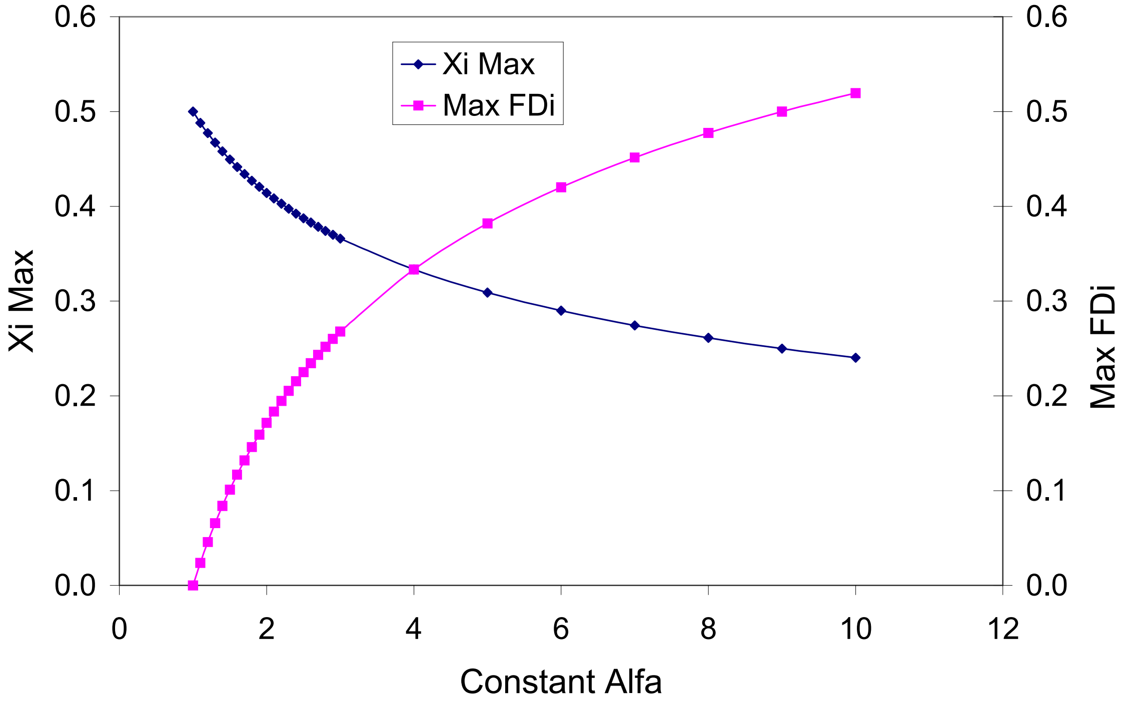


Figure 2: Plot of largest driving force, and the corresponding location of it as function of alfa.

Figure 2 can be used together with Table 1 to do a retrofit design, when the number of stages and desired product purities are known by the user. By following algorithm R1, one in principle moves from the right side of Table 1 towards the left side. One knows the number of stages and the desired product purities, this then gives the minimum reflux ratio, which then again gives the driving force available. Once the driving force is known, the range of alfas α can be found from Figure 2. In Table 1, a value for C = 1.5 has been applied., where C is the multiplication factor of RR to RRmin.

The algorithms presented here can be joined in a schematic framework for synthesis, design and retrofit. This framework is illustrated in Figure 3. Here the algorithms are divided into synthesis and retrofit algorithms in the first level. Then in the second level, the different synthesis steps are given, and one needs to decide what steps are necessary, and there will be an algorithm associated to it. In each algorithm, it is then specified what is given as input to the algorithm, and what the output from it is. In this way it is easy to get a clear overview of what is needed to apply this technique in a systematic way.

Table 1: Corresponding values of reflux ratio, minimum reflux ratio, number of stages, product purities and driving force

$FDi\|_{Max}$	$X_{LK,Dist}$	$X_{LK,Bot}$	RR_{Min}	RR_{Min}*C	N_{ideal}
0.045	0.995	0.005	9.89	14.83	96
	0.98	0.02	9.56	14.36	71
	0.95	0.05	8.9	13.35	54
	0.90	0.10	8.22	12.33	41
0.065	0.995	0.005	7.33	11.0	67
	0.98	0.02	7.10	10.65	50
	0.95	0.05	6.64	9.96	38
	0.90	0.10	5.72	8.58	29
0.101	0.995	0.005	4.50	6.74	44
	0.98	0.02	4.35	6.52	33
	0.95	0.05	4.05	6.08	25
	0.90	0.10	3.56	5.33	19
0.146	0.995	0.005	2.94	4.41	31
	0.98	0.02	2.84	4.26	23
	0.95	0.05	2.63	3.95	18
	0.90	0.10	2.29	3.44	14
0.172	0.995	0.005	2.35	3.53	27
	0.98	0.02	2.26	3.40	20
	0.95	0.05	2.09	3.13	15
	0.90	0.10	1.80	2.70	12
0.195	0.995	0.005	2.06	3.09	24
	0.98	0.02	1.98	2.97	18
	0.95	0.05	1.82	2.74	14
	0.90	0.10	1.57	2.35	11
0.225	0.995	0.005	1.73	2.60	21
	0.98	0.02	1.67	2.50	16
	0.95	0.05	1.53	2.30	12
	0.90	0.10	1.37	1.97	9
0.268	0.995	0.005	1.37	2.06	18
	0.98	0.02	1.31	1.97	13
	0.95	0.05	1.20	1.80	10
	0.90	0.10	1.02	1.52	8
0.382	0.995	0.005	0.82	1.23	13
	0.98	0.02	0.78	1.17	10
	0.95	0.05	0.70	1.05	8
	0.90	0.10	0.57	0.86	6
0.478	0.995	0.005	0.54	0.81	10
	0.98	0.02	0.51	0.76	8
	0.95	0.05	0.44	0.67	6
	0.90	0.10	0.34	0.51	5

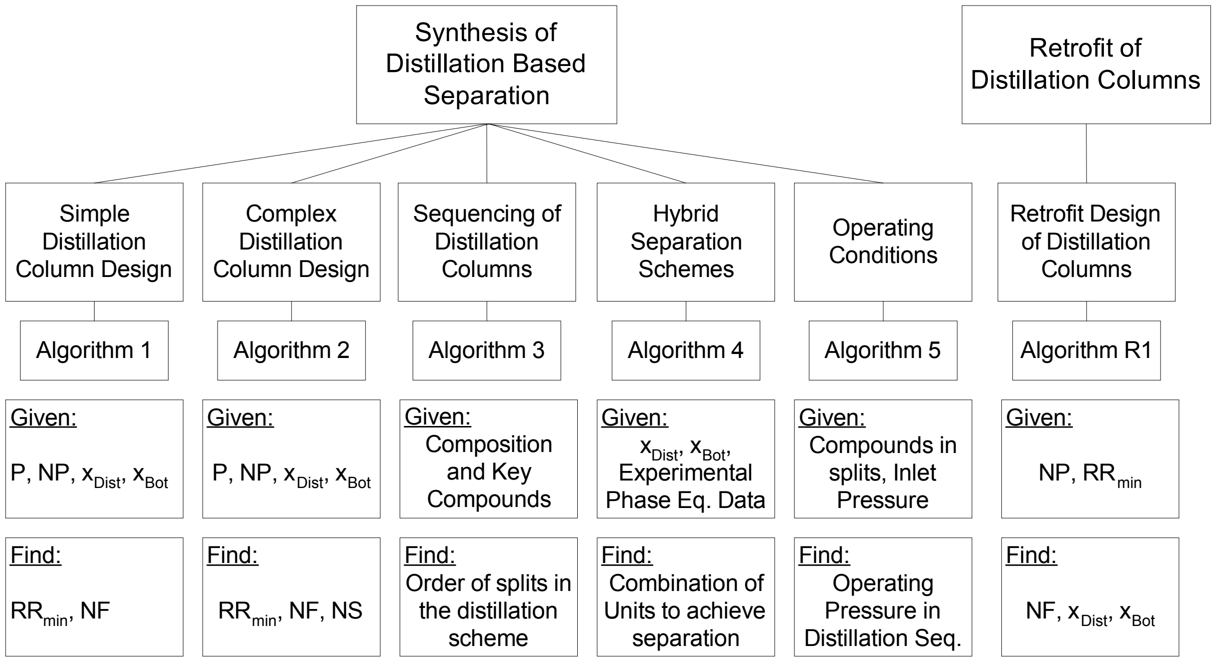


Figure 3: Framework for synthesis, design and retrofit, connecting the algorithms presented.

APPLICATIONS

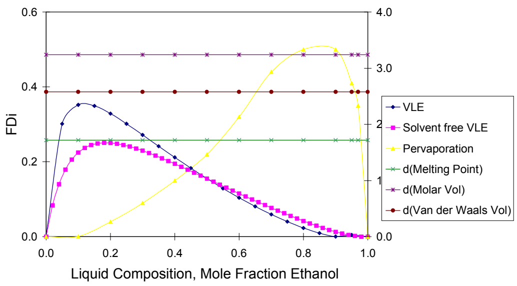
Applicability and scope of the driving force based algorithms are illustrated by a number of application examples. Especially algorithm 1 has been tested with many binary and multi-component mixtures some of which have been highlighted in [3]. These examples show clearly that the minimum energy consumption corresponds to NF located on the line D_y-D_x. In all these examples the energy consumption has been calculated for the following specified variables, NP, NF, A, B, and feed condition Examples of algorithm 3 are given in [1] where one example verifies the sequence of distillation columns of an optimisation study on an industrial plant. In [2] there is, among others also given an example of algorithm 3, where a sequence of 6 distillation columns is determined, and compared to an optimisation study. In [2] is also given examples of algorithms 4 and 5.

In the context of this paper, the focus will be aimed at the most recent developments in the proposed framework. One example of algorithm 4 will be given, but otherwise the focus will be on the algorithms on complex distillation design and retrofit design, i.e. algorithm 2 and R1. In each example an appropriate property model has been used to determine the driving force as a function of composition and the algorithms have been followed accordingly. For algorithm 2, a large number of examples have been worked out. This is partly due to the fact that the same systems have been applied for various feed compositions. This is also illustrated in example 2. The design has then been verified through rigorous simulation with the steady state distillation model in PRO/II. To present the results clearly to the reader, the examples given here will be given in individual sheets, where the steps of each algorithm can be followed easily.

Example 1: Separation of ethanol and water.

This is a well-known example of separation of ethanol and water. The example serves to illustrate algorithm 4. In the figure given in table 2, there are given driving force curves for 3 different 2-phase separation techniques. These are then compared throughout the range of composition in the separation, and the combination of separation techniques exhibiting the largest total driving force is identified. As indicated in Table 2, the combination of distillation with a membrane unit for pervaporation clearly is more efficient considering only energy consumption during operation.

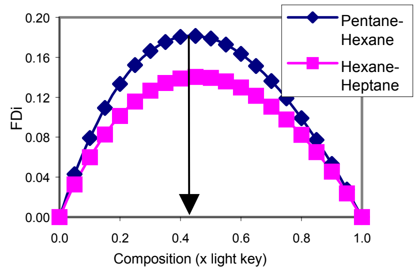
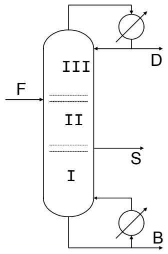
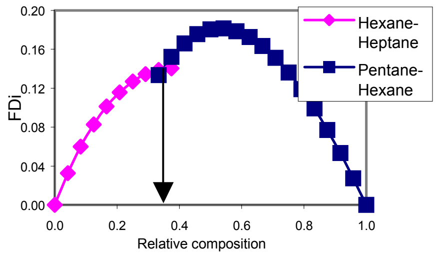
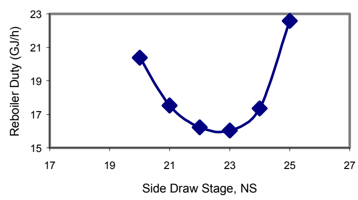
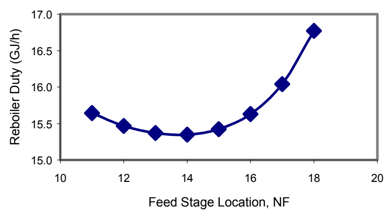
Table 2: Datasheet for example 1

Algorithm	Action	
Step 1 and 2	Identify azeotrope and retrieve data for different separation techniques.	
Step 3	Each component must be near unity in composition, (thus the azeotrope must be broken). Identify feasible paths	
Step 4	Identify separation techniques for each feasible path.	Alternatives: 1) Distillation and pervaporation, or 2) distillation with solvent, or 3) distillation with solvent and pervaporation.
Step 5	Choose combination with largest driving force	A hybrid flowsheet of distillation combined with pervaporation is chosen as initial flowsheet.
Validation		
Step 1	Identification of alternatives	Distillation + pervaporation Add solvent to distillation
Step 2	Rigorous calculation of energy duties	Distillation and pervaporation consumes maximum 73 % of the energy for a distillation column and a solvent recovery column.

Example 2: Separation of 3 hydrocarbons.

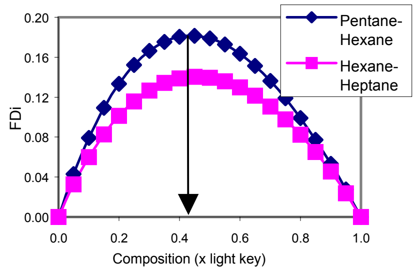
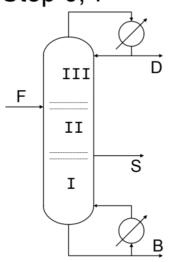
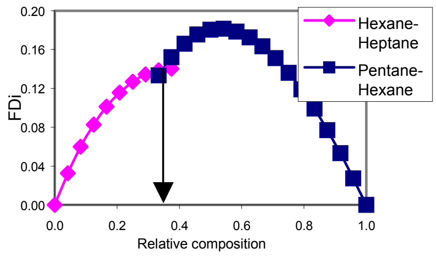
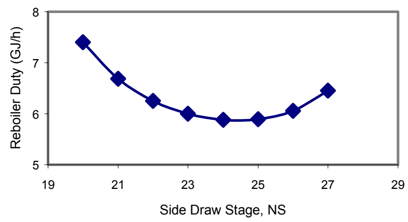
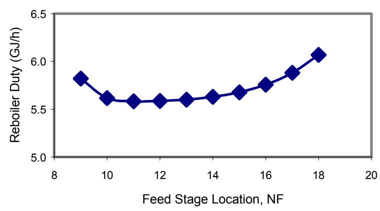
In this example, the separation of pentane, hexane and heptane in one column is considered. Tedder and Rudd [4] studied this system in the context of complex distillation design. There are two scenarios treated in this example, one where the feed mixture contains hexane (90 %) and 5 % of each of the two other compounds, and one where the feed is nearly equimolar. In both cases it is given that the columns operate at 5 atmosphere pressure and have 36 stages. The two driving force diagrams for this system are given as figures in tables 3 and 4. It is clearly seen that the pentane-hexane split is the easier split. Therefore this split is done first followed by a stripping section to the column to perform the split between hexane and heptane, as shown in sketch of the column under step 6, 7 in tables 3 and 4.

Table 3: Datasheet for example 2a.

Algorithm	Action	Problem 1 Feed (0.05, 0.90, 0.05)
Step 1, 2, 3, 4 , 5	Calculate 2 FD curves Dx = 0.45 Pentane-Hexane exhibits the larger driving force.	
Step 6, 7 	Generate Joint curve Ds = 0.32	
Step 8	Give number of stages	N = 36 (Given already)
Step 9	Determine RRmin	2.02
Step 10a	Give Spec 1	XD (Pentane) = 0.998
Step 10b	Give Spec 2	XB (Heptane) = 0.85
Step 10c	Determine Side draw	Side draw = Feed * 0.90
Step 11	Determine N_S	N_S = 36(1-0.32) = 24.48 ~ 24
Step 12	Determine N_F	N_F = 24(1-0.45) = 13.2 ~ 13
Validation		
Step 1	Simulation for various N_S Ns opt. = 23	
Step 2	Simulation for various N_F Nf opt. = 14	
Step 3	Actual RR / V/F	116.7 / 5.78

When the order of the splits has been determined, the actual positions of the feed and the side-draw are determined accordingly. The results of the predictions have been verified with rigorous simulation as indicated in tables 3 and 4.

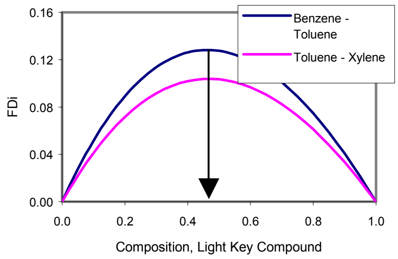
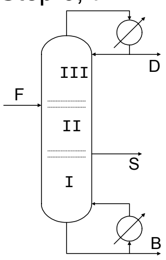
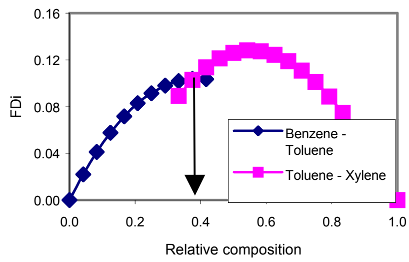
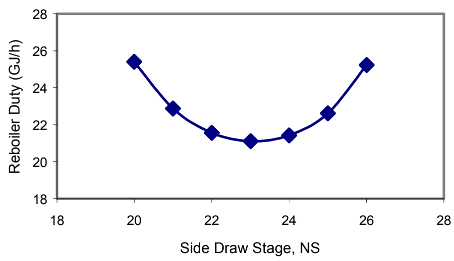
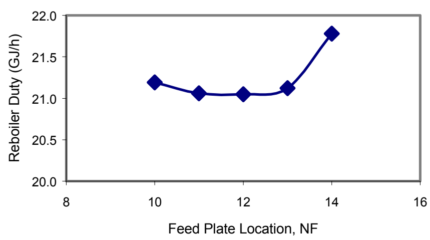
Table 4: Datasheet for example 2b.

Algorithm	Action	Problem 1 Feed (0.34, 0.33, 0.33)
Step 1, 2, 3, 4, 5	Calculate 2 FD curves Dx = 0.45	
Step 6, 7 	Generate Joint curve Ds = 0.32	
Step 8	Give number of stages	N = 36 (Given already)
Step 9	Determine RRmin	2.02
Step 10a	Give Spec 1	XD (Pentane) = 0.998
Step 10b	Give Spec 2	XB (Heptane) = 0.85
Step 10c	Determine Side draw	Side draw = Feed * 0.33
Step 11	Determine N_S	N_S = 36(1-0.32) = 24.48 ~ 24
Step 12	Determine N_F	N_F = 24(1-0.45) = 13.2 ~ 13
Validation		
Step 1	Simulation for various N_S Ns opt. = 24	
Step 2	Simulation for various N_F Nf opt. = 12	
Step 3	Actual RR / V/F	4.91 / 1.67

<u>Example 3: Separation of BTX mixture.</u>

Another example is a classical separation problem, the mixture of benzene, toluene and xylenes. This mixture is also to be separated in a column with 3 product streams, and algorithm 2 has been applied. The column is specified to operate at 10 atmosphere pressure and has 40 stages. Just as in example 2, the steps of the algorithm are presented in schematic form in Table 5.

Table 5: Datasheet for example 3

Algorithm	Action	Problem 1 Feed (0.33, 0.33, 0.34)
Step 1, 2, 3, 4, 5	Calculate 2 FD curves Dx = 0.46	
Step 6, 7 	Generate Joint curve Ds = 0.38	
Step 8	Give number of stages	N = 40 (Given already)
Step 9	Determine RRmin	3.28
Step 10a	Give Spec 1	XD (Benzene) = 0.995
Step 10b	Give Spec 2	XB (Xylene) = 0.92
Step 10c	Determine Side draw	Side draw = Feed * 0.33
Step 11	Determine N_S	N_S = 40(1-0.38) = 24
Step 12	Determine N_F	N_F = 24(1-0.46) = 12.96 = 12/13
Validation		
Step 1	Simulation for various N_S Ns opt. = 23	
Step 2	Simulation for various N_F Nf opt. = 12	
Step 3	Actual RR / V/F	21.7 / 7.13

Example 4: Retrofit design.

This is an example of the retrofit algorithm, R1. Here we are dealing with a column of 60 stages, and we have options to feed on stages 33 and 38. The procedure is followed, making use of table 1, and figure 2. The results of the example are listed in Table 6. With the given product specifications, and the corresponding driving force, immediately 3 mixtures suitable for separation in this column were found.

Table 6: Datasheet for example 4

Algorithm	Action	
Step1	Determine desired products	$X_{B,\ HK}$ = 0.995 $X_{D,\ LK}$ = 0.995
Step 2	Find F_{DiMax}	~ 0.07
Step 3	Find range of α	α ~0.33-0.34
Step 4	Find, RR_{min},	RRmin ~ 6.4
Step 5	Check for mixtures with these properties	1) Butane-iButane, 5 atm. 2) Cycloheptanol-Cycleoctanol, 5 atm 3) 1,4Butanediol-1,3Butanediol, 15 atm 4) Hexanol-Hexanal, 12 atm 5) DiethyleneGlycol-1,6-Hexanediol, 3 atm
Verification		
Mixture 1	Butane-iButane, 5 atm	α ~ 1.33-1.34 FDi ~ 0.074
Mixture 2	Cycloheptanol-Cyclo-octanol, 5 atm	α ~ 1.34-1.38 FDi ~ 0.080
Mixture 3	1,4Butanediol-1,3Butanediol, 15 atm	α ~ 1.3-1.85 FDi ~ 0.065-1.45
Mixture 4	Hexanol-Hexanal, 12 atm	α ~ 1.24-1.57 FDi ~ 0.05-1.0
Mixture 5	DiethyleneGlycol-1,6-Hexanediol, 3 atm	α ~ 1.22-1.34 FDi ~ 0.05-0.07

CONCLUSIONS

An integrated framework for synthesis and design of distillation based separation systems has been proposed. The framework is based on the driving force approach [3] and further extends it, enabling thereby solution of a wide range of problems. The framework consists of six algorithms that in an integrated manner enable the visual determination of the near-optimal (if not optimal) separation sequences together with the corresponding condition of operation and design for both conventional and complex distillation columns. The integrated approach is also able to generate hybrid separation schemes where different separation techniques are allowed. With this approach, the only requirements for the integrated framework are co-existing phase composition data. The approach requires no rigorous simulation or optimisation. The methodology not only identifies the feasibility of different separation techniques for a given separation task, but also indicates the optimum methods of separation. Consequently, it is possible to make early decisions on separation sequences and distillation configurations that are near-optimum solutions. Also, the original driving force approach is now extended to handle complex distillation columns. It is evident that this extended methodology is able to generate near optimum designs of even very complicated distillation columns, based on the simple and visual techniques. Finally, the results appear to confirm the theory that separation at the highest driving force is the easiest separation and therefore, should require a near minimum of energy. Since energy is needed to create the driving force, this conclusion is not surprising.

NOMENCLATURE

A	Product composition specification (see figure 1)
B	Product composition specification (see figure 1)
C	Multiplication factor for RRmin to RR
D	Largest driving force
Ds	Relative position of side-draw driving force
Dx	Relative position of largest driving force
Dy	Size of largest driving force
F	Feed [Kmole/hr]
F_{ij}, FDi	Driving force
HK	Heavy key compound
LK	Light key compound
RR	Reflux ratio
RRmin	Minimum reflux ratio
N	Number of stages
N_F	Feed stage
N_P	Number of stages
N_S	Side draw stage
P	Pressure [Atmosphere]
T	Temperature [Kelvin]
x_i	Liquid composition of compound i
y_i	Vapour composition of compound i
α	Relative volatility
β	Relative separability
θ	Resistance factor

Subscripts:

B, Bot	Bottom composition
D, Dist	Distillate composition
Z	Feed composition

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