A NOVEL FRAMEWORK FOR SIMULTANEOUS SEPARATION PROCESS AND PRODUCT DESIGN

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ABSTRACT

The objective of this paper is to introduce a systematic framework for simultaneous solution process/product design problems related to separation. This framework is based on the recently developed property clustering approach that allows one to perform design calculations on a component-free (or composition-free) basis. Removing the composition dependency from the design problem enables the simultaneous consideration of process and product selection and optimization. The clustering concept is based on the observation that properties, unlike mass, are not conserved and consequently they cannot be tracked among process units without performing component material balances. To overcome these limitations the use of conserved property-based clusters has been proposed. The model derivations and reformulations to cluster-based models are presented and the usage highlighted through a simple proof of concept example and a case study.

INTRODUCTION

Aside from reaction systems, the primary task of most processing units is to tailor properties of various streams throughout the process. Furthermore, the use of streams and species throughout the process is primarily driven by the need to satisfy certain properties in the processing units. Notwithstanding the critical role of properties in designing a process, the conventional approach to process design is based on tracking mass and energy throughout the process. Properties are considered indirectly by selecting species as well as operating conditions and ensuring that the resulting properties are acceptable. This approach is quite limiting since the insights associated with properties are masked by species and operating conditions. Alternatively, properties should be tracked and integrated explicitly. The framework for property integration has been presented recently [1, 2, 3] and is based on existing property clustering techniques [4]. It is a holistic approach to the tracking, manipulation, and allocation of properties throughout the process. A process can be represented through sources, sinks, and interception devices as shown in Figure 1. Sources are process streams that possess certain properties. Sinks are process

units that process the sources. Interception devices are additional units that can modify the properties of the sources. Property integration deals with the identification of optimal mixing, splitting, segregation, and interception of sources so as to satisfy the property constraints for the sinks. The application range of the original clustering approach is extended by deriving cluster based unit operation models. The models are derived from the fundamental process models and reformulated with respect to clusters. The objective being to replace component based material balances with cluster based material balances without any simplification or loss of information. Another advantage of the clustering concept is that, by removing the compositions as variables, even a large dimension problem solution can be visualized in the two- or three-dimensional space.

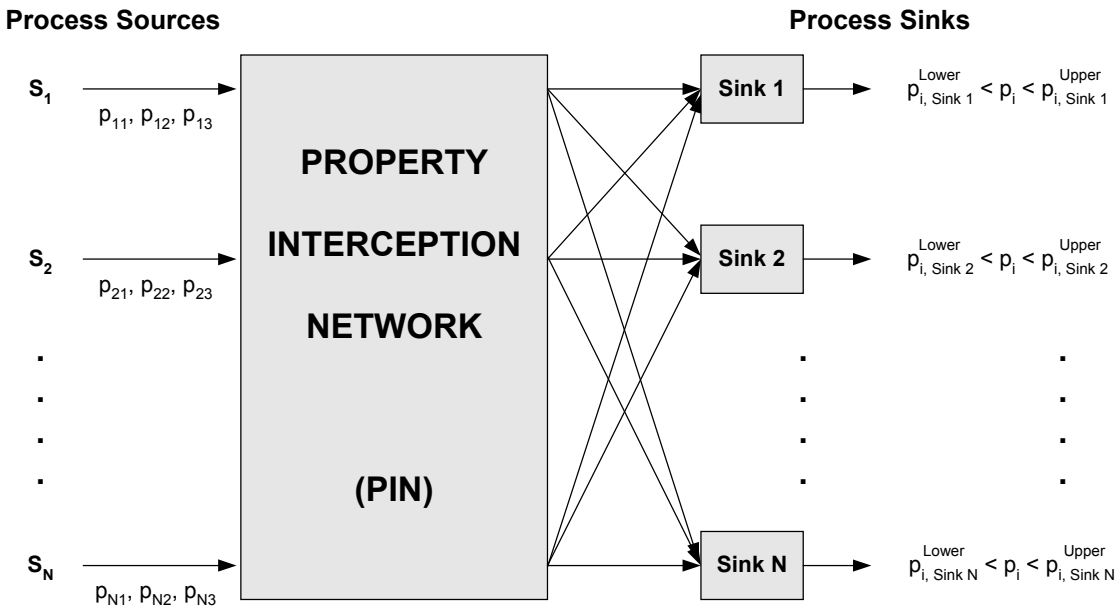

Figure 1: Schematic representation of property integration framework

Design of compounds with specified properties is a typical example of product/process design problems, where the clusters together with their target properties are first determined and then molecules (and/or mixtures) that satisfy the targets are determined. In this integrated problem, the process target values are used to generate product data while the product target values are used to generate the process data. The scope of this approach is potentially very large - from simultaneous design and selection of heat exchangers and process fluids to mass exchangers and solvents/agents. This methodology may be employed to design novel separation schemes involving distillation and adsorption processes by removing the composition dependency from the problem, thus yielding the property targets for the components to be separated. Once the property targets have been identified, the corresponding components may be identified using molecular design techniques.

PROCESS AND PRODUCT DESIGN ISSUES

Traditionally process design and molecular design have been treated as two separate problems, with little or no feedback between the two approaches. Each problem has been conveniently isolated or decoupled from the other. Figure 2 shows a schematic representation of the two problems, e.g. the required inputs and solution objectives of the different design algorithms. Both approaches have some inherent limitations due to the amount of information that is required prior to invoking the design algorithm. When considering conventional process design methodologies, the selected species are chosen from among a list of pre-defined candidate components, therefore, limiting performance to the listed components. On the other hand, with molecular design techniques, the desired target properties are required input to the solution algorithm. Once again these decisions are made ahead of design and are usually based on qualitative process knowledge and/or experience and thus possibly yield a sub-optimal design.

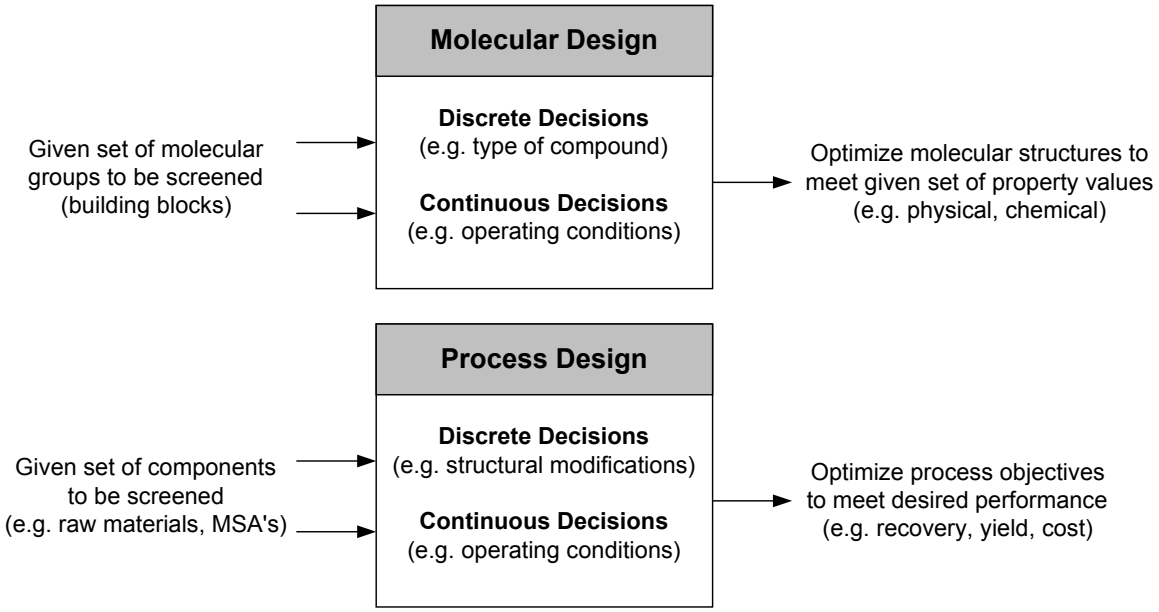

Figure 2: Conventional solution approach for process and molecular design problems

To overcome the limitations encompassed by decoupling the process and molecular design problems, a simultaneous approach as outlined in Figure 3 is proposed. Using this approach the necessary input to the methodology is the molecular building blocks and the desired process performance, for the molecular and process design algorithms respectively. The final outputs of the algorithm are the design variables, which facilitate the desired process performance target and the molecules that satisfy the property targets identified by solution of the process design problem. The strength of this approach is to identify the property values that correspond to the optimum process performance without committing to any components at this stage. This is a critical characteristic for property integration. These property values are then used for the molecular design, which returns the corresponding components. One inherent problem with this approach is the need to solve the process design problem in terms of properties and not components.

The conventional decoupled solution methodology presented in Figure 2 can be described as a “forward” problem formulation, whereas the simultaneous solution approach given in Figure 3 consists of solving two “reverse” problems. Solving the process design problem in terms of properties corresponding to the desired process performance identifies the design targets. In principle this part is the reverse of a simulation problem. Similarly solution of the molecular design problem to identify candidates that match the optimal design targets is the reverse of a property prediction problem. By employing this reverse problem formulation approach an inherent benefit is that the constitutive model equations are decoupled from the mass and energy balance equations, thus making the solution of the problem very easy. The reasoning behind this is that all solutions matching the design targets also satisfy the mass and energy balances; therefore it is not necessary to resolve the balance equations for all design alternatives. Once the targets have been identified the constitutive equations are solved to find the parameters and/or components required to match the targets.

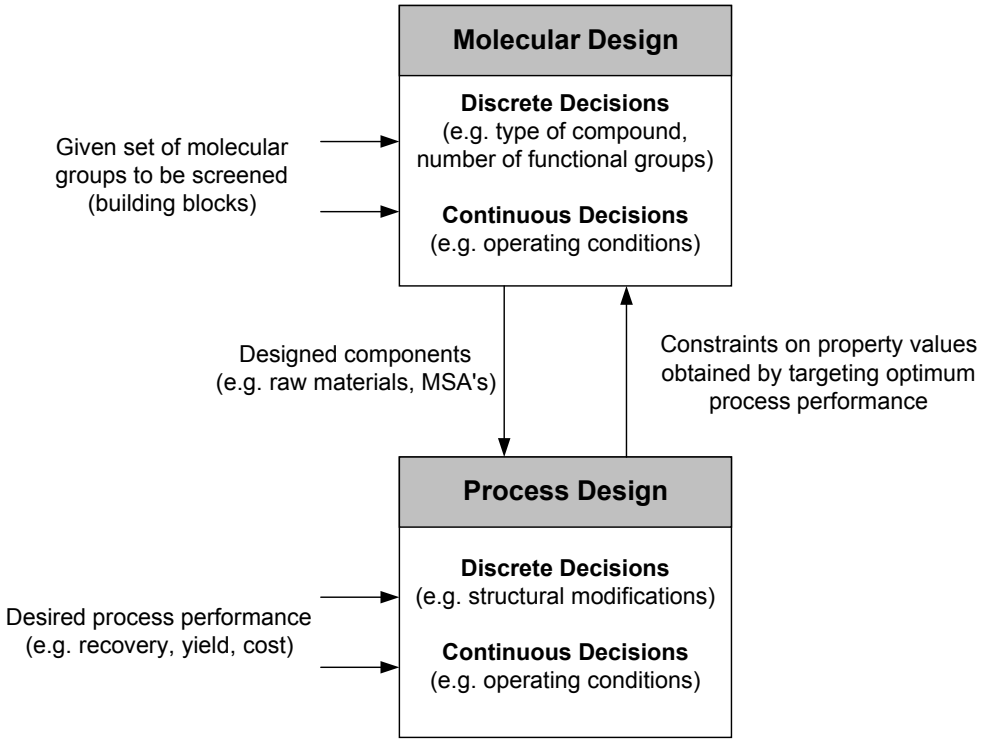

Figure 3: New approach for simultaneous solution of process and molecular design problems

Unfortunately properties, unlike mass and energy, are not conserved; hence a framework for tracking properties among process streams and process units is needed.

GENERAL PROBLEM FORMULATION

A general process/product synthesis and/or design problem can be represented in generic terms by the following set of equations:

$$F_{Obj} = \min\{C^T y + f(x)\} \qquad (1)$$

s.t. $h_1(x,y) = 0$ (2)

$h_2(x,y) = 0$ (3)

$g_1(x) > 0$ (4)

$g_2(x,y) > 0$ (5)

$B \cdot y + C \cdot x > d$ (6)

In the above equations, F_{Obj} is the objective function that needs to be minimized or maximized in order to satisfy the desired performance criteria; x and y are the optimization real and integer variables respectively; h_1 represents the process model equations; h_2 represents process equality constraints; g_1 and g_2 represent other process/product related inequality constraints, while equation (6) represents structural constraints related to process as well as products.

It is important to point out, that all synthesis/design problems may be described using this generalized set of equations. Depending on the specific problem some terms and equations may be omitted, e.g. determination of only feasible solutions will not require equation (1). It must be emphasized however, that regardless of the problem a process model represented by equation (2) is needed and it is the model type and validity ranges that defines the application range of the solution. Hence heuristic and graphical methodologies resulting in a feasible but not necessarily optimal solution, as well as mathematical programming techniques that determine optimal solutions can be formulated and solved by defining equations (1)–(6).

REVERSE PROBLEM FORMULATION

In principle the process model equations consist of balance equations, constraint equations and constitutive equations [5]. The model type and complexity is implicitly related to the constitutive equations, hence decoupling the constitutive equations from the balance and constraint equations will in many cases remove the model complexity. These considerations are the foundation for two reverse problem formulations:

1. Given input stream(s) variables, equipment parameters and known output stream(s) variables, determine the constitutive variables.

2. Given values of the constitutive variables, determine the unknown intensive variables (from the set of temperature, pressure and composition) and/or compound identity and/or molecular structure.

The first problem above is the reverse of a simulation problem, i.e. it determines the design targets for a given set of specified inputs and outputs. The second problem matches the calculated targets, for the process conditions, process flowsheets or products (including molecular structure). As long as the targets are matched, the process model equations (minus the constitutive equations) do not need to be solved again.

It should be emphasized that optimization problems based on reverse simulation problems, are not limited by the application range or complexity of the constitutive equations. Therefore the solution is easy and can be visualized. Another advantage is that for the second reverse problem, any number of independent models may be used, as long as they match the target constitutive variable values. This implies that more than one process and/or product can be identified by matching the design targets, thus it is possible to determine all feasible solutions. Once the feasible solutions have been identified, the optimal solution may be found by ranking the solutions according to a performance index. It is important to point out that the solution strategy presented below is valid for new process synthesis/design problems as well as retrofit problems. The different problem types define the choice of equations and variables.

GENERAL SOLUTION STRATEGY

The methodology for solving the integrated process and product design problems is divided in three parts. Below the different steps of the method are presented, steps 1 and 2 constitute the input specification and model generation steps, step 3 formulates and solves the reverse simulation problem, while step 4 solves the reverse property prediction problem. Finally step 5 identifies the optimal solution by employing a ranking approach.

1. Specify the synthesis/design problem in terms of known inputs and known outputs (for new process and product) and/or equipment parameters (for retrofit problems).

2. Select the unit operations to be considered and generate the corresponding individual process models (without the constitutive equations).

3. Formulate and solve the reverse simulation problem with the constitutive variables as the unknown (design) variables that match a specified design target (can be solved as optimization problem or simply as a reverse simulation problem).

4. Formulate and solve the reverse property prediction problem in order to determine the conditions of operation, flowsheet structure and/or product that match the target values identified in step 3.

5. Compute the performance index for all feasible solutions from step 4 and order them to determine the optimal solution.

DEFINITION OF PROPERTY CLUSTERS

To overcome the limitations encompassed when trying to track properties among process streams and units, the use of conserved property-based clusters has been proposed [4]. The clusters are tailored to possess the two fundamental properties of inter- and intra-stream conservation, thus enabling the development of consistent additive rules along with their ternary representation. The clusters are obtained by mapping property relationships into a low dimensional domain, thus allowing for visualization of the problem. The clusters can be described as conserved surrogate properties, which are functions of the raw properties. The clustering approach utilizes property operators defined as:

$$\psi_j(P_{jM}) = \sum_{s=1}^{N_s} \frac{F_s}{\sum_{s=1}^{N_s} F_s} \cdot \psi_j(P_{js}) \tag{7}$$

The property operator formulation allows for simple linear mixing rules, i.e. the operators correspond to the actual properties, or the operators may describe functional relationships of the properties, e.g. for density, where the resulting property of mixing two streams is given as the inverse of the summation over the reciprocal property values multiplied by their fractional contribution. The property operators are converted to dimensionless variables by division by an arbitrary reference, which is appropriately chosen such that the resulting dimensionless properties are of the same order of magnitude:

$$\Omega_{js} = \frac{\psi_j(P_{js})}{\psi_j^{ref}} \tag{8}$$

An Augmented Property index (AUP) for each stream *s* is defined as the summation of all the dimensionless property operators:

$$AUP_s = \sum_{j=1}^{NP} \Omega_{js} \tag{9}$$

The property cluster for property *j* of stream *s* is defined as:

$$C_{js} = \frac{\Omega_{js}}{AUP_s} \tag{10}$$

Incorporating these clusters into the mass integration framework [5] enables the identification of optimal strategies for recovery and allocation of plant utilities. Process insights are obtained through visualization tools based on optimization concepts. Since the clusters are tailored to maintain the two fundamental rules for intra- and inter-stream conservation, lever-arm analysis may be employed extensively to identify recycle potentials [6, 7]. For visualization purposes the number of clusters is limited to three, however when using mathematical programming this limitation is removed.

MODEL DERIVATIONS

In order to utilize the possibilities of visualizing process synthesis/design problems by means of property clusters it is necessary to have models for different unit operations reformulated in terms of such clusters. In the following the fundamental composition based balance models are derived and reformulated to obtain cluster based models, which satisfy the original mass balance equations. In this contribution the models are derived for mixing and splitting only, thus covering separation and recycle problems. Current efforts are focused on extending the methodology to include reactive systems as well.

Cluster Formulation of Mixer Model

Any mixing operation can be described by a series of binary mixing processes, i.e. where two feed streams are mixed to obtain one product stream.

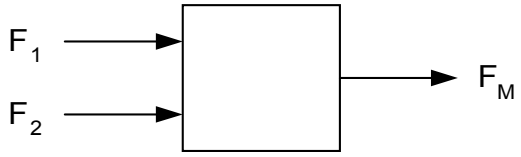

Figure 4: Mixer schematic

The individual component balances for component *i* may be written as:

$$F_1 \cdot y_{i1} + F_2 \cdot y_{i2} = F_M \cdot y_{iM} \tag{11}$$

Introducing a mixture flowrate fraction and rearranging to find the mixture compositions:

$$y_{iM} = \beta_{Mix} \cdot y_{i1} + (1-\beta_{Mix}) \cdot y_{i2} \quad , \beta_{Mix} = \frac{F_1}{F_M}, \quad 1-\beta_{Mix} = \frac{F_2}{F_M} \tag{12}$$

The foundation of the cluster-based description of any system is the ability to adequately describe all the streams by a finite number of *j* properties. For visualization purposes only 3 properties are used. Equation (12) can be rewritten in terms of dimensionless property operators as follows:

$$\Omega_{jM} = \beta_{Mix} \cdot \Omega_{j1} + (1-\beta_{Mix}) \cdot \Omega_{j2} \tag{13}$$

The AUgmented Property index for the mixture can be calculated by summation of the dimensionless property operators, as defined by equation (9):

$$AUP_M = \beta_{Mix} \cdot AUP_1 + (1-\beta_{Mix}) \cdot AUP_2 \tag{14}$$

Equation (14) shows that a lever-arm rule exists for calculating the AUP index for a mixture of two streams using only the feed stream properties. Employing the cluster definition given in equation (10) the mixture clusters may be calculated. Combining equations (10) and (13) yields:

$$C_{jM} = \beta_{Mix} \cdot \frac{AUP_1}{AUP_M} \cdot C_{j1} + (1-\beta_{Mix}) \cdot \frac{AUP_2}{AUP_M} \cdot C_{j2} \qquad (15)$$

Once again a lever-arm expression is obtained to determine the cluster values of the mixture using only the feed stream information. This was a desired feature of the clusters (inter-stream conservation), as it provides the option of consistent additive rules to be used within a ternary representation of the problem. It must be emphasized at this point that the cluster based mixing model represented by equation (15) originates from the original mass balance equation, thus any design calculations carried out using equation (15) will satisfy the mass balance.

Table 1: Calculation sequence for identification of mixture clusters

Step	Description	Equation
Mix1	Calculate dimensionless feed stream property values	(8)
Mix2	Calculate feed stream AUP indices	(9)
Mix3	Calculate ternary cluster values for each feed stream	(10)
Mix4	Calculate flowrate distribution	(12)
Mix5	Calculate AUP index for the mixture	(14)
Mix6	Calculate ternary cluster values for the mixture	(15)

Once the mixing operation has been solved in the cluster domain, the result must be converted back to the property domain and finally the corresponding compositions must be identified. After the conversion to properties the following equation, where each property *j* of the mixture is a function of composition, is given:

$$\Omega_{jM} = f_j(y_{iM}) \quad , i \in [1, NC] \qquad (16)$$

Furthermore the compositions of the mixture must sum to unity:

$$\sum_{i=1}^{NC} y_{iM} = 1 \qquad (17)$$

A degree of freedom analysis of the system shows that the number of variables (unknowns) is NC, while the number of equations is j+1. Thus the degrees of freedom are NC–(j+1). This means that for NC>j+1 the system cannot be uniquely solved. The reason for this result is that a high dimensional system is mapped to a system of only j dimensions. When trying to return to the composition space for NC > j + 1, the solution is not unique, since infinite parameter combinations exist that obey the above equations.

However only ONE solution exists that also satisfies the mass balance equations. Therefore by fixing NC–(j+1) compositions from the mass balance equations, this unique solution of the original NC x NC system is guaranteed. Any set of components may be chosen for which to fix the compositions, however in order to have a common rule base, the components $i \in$[j+2, NC] are chosen.

It should be noted that by including the mass balance equations as constraints, the above described problem could also be solved uniquely by mathematical optimization.

Cluster Formulation of Splitter Model

A procedure analogous to the one performed on the fundamental mixer model, can be performed for a component splitter unit. Any splitting operation can be described by a series of binary splitting processes, i.e. where one feed stream is split to obtain two product streams.

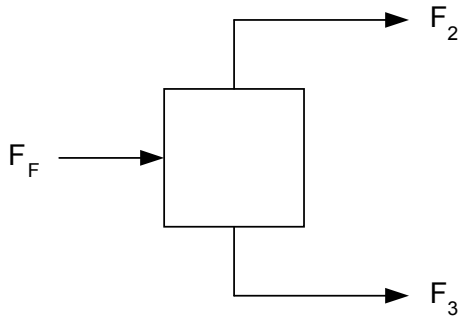

Figure 5: Splitter schematic

The individual component balances for component *i* may be written as:

$$F_F \cdot y_{iF} = F_2 \cdot y_{i2} + F_3 \cdot y_{i3} \tag{18}$$

Introducing a product flowrate fraction and rearranging yields:

$$y_{iF} = \beta_{Split} \cdot y_{i2} + (1-\beta_{Split}) \cdot y_{i3} \quad , \beta_{Split} = \frac{F_2}{F_F}, \quad 1-\beta_{Split} = \frac{F_3}{F_F} \tag{19}$$

We now introduce the component split factors:

$$S_i = \frac{F_2 \cdot y_{i2}}{F_F \cdot y_{iF}} \quad \Leftrightarrow \quad S_i \cdot y_{iF} = \beta_{Split} \cdot y_{i2} \tag{20}$$

Summation over all components yields the product flowrate fraction:

$$\sum_{i=1}^{NC} S_i \cdot y_{iF} = \beta_{Split} \cdot \sum_{i=1}^{NC} y_{i2} \quad \Leftrightarrow \quad \beta_{Split} = \sum_{i=1}^{NC} S_i \cdot y_{iF} \tag{21}$$

Combining equations (19) and (20) yields:

$$y_{iF} = S_i \cdot y_{iF} + (1-\beta_{Split}) \cdot y_{i3} \tag{22}$$

For visualization purposes only 3 properties are used. Equation (19) can be rewritten in terms of dimensionless property operators as follows:

$$\Omega_{jF} = \beta_{Split} \cdot \Omega_{j2} + (1-\beta_{Split}) \cdot \Omega_{j3} \tag{23}$$

A similar expression can be obtained by reformulating equation (22) in terms of dimensionless property operators:

$$\Omega_{jF} = \Omega_{jFSplit} + (1-\beta_{Split}) \cdot \Omega_{j3} \tag{24}$$

In equation (24) a pseudo dimensionless property operator $\Omega_{jFSplit}$ is introduced. This parameter describes the relationships between the properties of product stream 2 as a function of the properties of the feed stream. It should be noted that $\Omega_{jFSplit}$ is a function of known variables only, i.e. the split factors, feed stream composition and the pure component property values, and in principle $\Omega_{jFSplit}$ can be described as a property split factor. This new parameter is easily calculated (the annotation for pure component properties, which are marked by a *, uses two indices, i.e. *j* is the property ID, while *i* denotes the component ID):

$$\Omega_{jFSplit} = \sum_{i=1}^{NC} \Omega_{ji}^{*} \cdot S_i \cdot y_{iF} \tag{25}$$

Equation (24) can be rearranged to provide an expression for the properties of product stream 3:

$$\Omega_{j3} = \frac{\Omega_{jF} - \Omega_{jFSplit}}{1-\beta_{Split}} \tag{26}$$

Inserting this expression in equation (23) provides the corresponding expression for the properties of product stream 2:

$$\Omega_{j2} = \frac{\Omega_{jFSplit}}{\beta_{Split}} \tag{27}$$

The AUgmented Property index for the two product streams can be calculated by summation of the dimensionless property operators, as defined by equation (9):

$$AUP_2 = \sum_j \Omega_{j2} = \sum_j \frac{\Omega_{jFSplit}}{\beta_{Split}} = \frac{1}{\beta_{Split}} \sum_j \Omega_{jFSplit} \tag{28}$$

$$AUP_3 = \sum_j \Omega_{j3} = \sum_j \frac{\Omega_{jF} - \Omega_{jFSplit}}{1-\beta_{Split}} = \frac{1}{1-\beta_{Split}} \sum_j (\Omega_{jF} - \Omega_{jFSplit}) \tag{29}$$

Employing the cluster definition given in equation (10) the product clusters may be calculated:

$$C_{j2} = \frac{\Omega_{j2}}{AUP_2} = \frac{\Omega_{jFSplit}}{\sum_j \Omega_{jFSplit}} \tag{30}$$

$$C_{j3} = \frac{\Omega_{j3}}{AUP_3} = \frac{\Omega_{jF} - \Omega_{jFSplit}}{\sum_j (\Omega_{jF} - \Omega_{jFSplit})} \quad (31)$$

An interesting feature of the splitter model is that the resulting product clusters are independent of the flowrate distribution even though the stream properties are functions of β_{Split}.

For a given set of component split factors S_i, the calculation sequence given in Table 2 yields the ternary cluster values for the two product streams. The sequence in Table 2 includes the calculation of the product stream properties and AUP indices as these are necessary for converting the solution back to composition space. It should be noted however that the product cluster values could have been calculated using only the feed stream information and the component split factors. This means that steps 6 and 7 in Table 2 are not required for the cluster based solution but generates the necessary data for the composition based solution.

Table 2: Calculation sequence for identification of product clusters from splitting operation

Step	Description	Equation
Split1	Calculate dimensionless feed stream property values	(8)
Split2	Calculate feed stream AUP index	(9)
Split3	Calculate ternary cluster values for feed stream	(10)
Split4	Calculate flowrate distribution	(21)
Split5	Calculate the property split factors	(25)
Split6	Calculate dimensionless property values for products	(26) & (27)
Split7	Calculate AUP index for product streams	(28) & (29)
Split8	Calculate ternary cluster values for product streams	(30) & (31)

By repeating the calculation sequence for all parameter combinations of S_i ranging from 0 to 1 in suitable intervals, e.g. with a step size of 0.1, the feasibility region for the splitting operation is obtained. It should be noted that the any separation technique and conditions of operation will result in ternary clusters within this region, thus it can be used for identifying the design targets, i.e. the set of separation factors.

Once the splitting operation has been solved in the cluster domain, the results must be converted back to the property domain and finally the corresponding compositions must be identified. After the conversion to properties the following equations, where each property *j* of the products is a function of composition, are given:

$$\Omega_{j2} = f_j(y_{i2}) \quad , i \in [1, NC] \quad (32)$$

$$\Omega_{j3} = f_j(y_{i3}) \quad , i \in [1, NC] \quad (33)$$

Furthermore the compositions in each product stream must sum to unity:

$$\sum_{i=1}^{NC} y_{i2} = 1 \quad (34)$$

$$\sum_{i=1}^{NC} y_{i3} = 1 \qquad (35)$$

A degree of freedom analysis of the system shows that the number of variables (unknowns) is 2*NC, while the number of equations is 2*(j+1). Thus the degrees of freedom are 2*NC–2*(j+1). It could be argued that since all the component split factors are known, the compositions of one product stream is also known. However to obtain square matrices, only the compositions for components $i \in [j+2, NC]$ are calculated by using the split factors. The corresponding compositions in the other product stream are fixed from the mass balance equations, thus yielding 2 NC x NC systems, which can be uniquely solved to obtain the product compositions.

ILLUSTRATIVE EXAMPLE

The problem to be solved involves choosing the correct sequence of mixers and splitters for matching a set of target values. It should be noted that the example is based on purely theoretical values, which are not related to any specific components or properties. The purpose of this example is solely to illustrate and validate the use of mixing and splitting operations for solving design problems in cluster space.

Problem Formulation

The objective is to match a set property values for a product stream by mixing and splitting two feed streams accordingly. Three properties P_1, P_2 and P_3 have been found to be able to characterize the streams. The initial inputs, i.e. pure component property values, property references, stream summaries as well as the desired property targets are given in Table 3 – Table 5 below.

Table 3: Pure component property data

Component i	Pure Component Properties		
	P^*_{1i}	P^*_{2i}	P^*_{3i}
1	50	1.2	10
2	65	0.5	8
3	38	0.8	12
4	100	2.0	4
5	118	0.2	3
6	75	0.5	12

Table 4: Feed stream summaries

Data	Feed Stream 1	Feed Stream 2
y_{1s}	0.1889	0.0000
y_{2s}	0.4667	0.0000
y_{3s}	0.3444	0.0000
y_{4s}	0.0000	0.1000
y_{5s}	0.0000	0.7500
y_{6s}	0.0000	0.1500
Flowrate	10.0	150.0

Table 5: Property targets and reference values

Property	Target Value	Reference Value
P_1	78.840	50
P_2	1.247	1
P_3	7.688	7

Visualization of Problem

Valuable insights may be obtained by visualizing the problem. Converting the feed stream and property target information to clusters is achieved by employing equations (8)–(10). The resulting cluster source-sink mapping is given in Figure 6. Since all mixing operations within the cluster diagram are described by a straight line, it is evident from Figure 6 that it is NOT possible to mix the two feed streams in any ratio to match the property targets. Therefore it is necessary to split at least one of the streams. The feasibility regions are identified by employing the calculation sequence outlined in Table 2 using a parameter step size of 0.1.

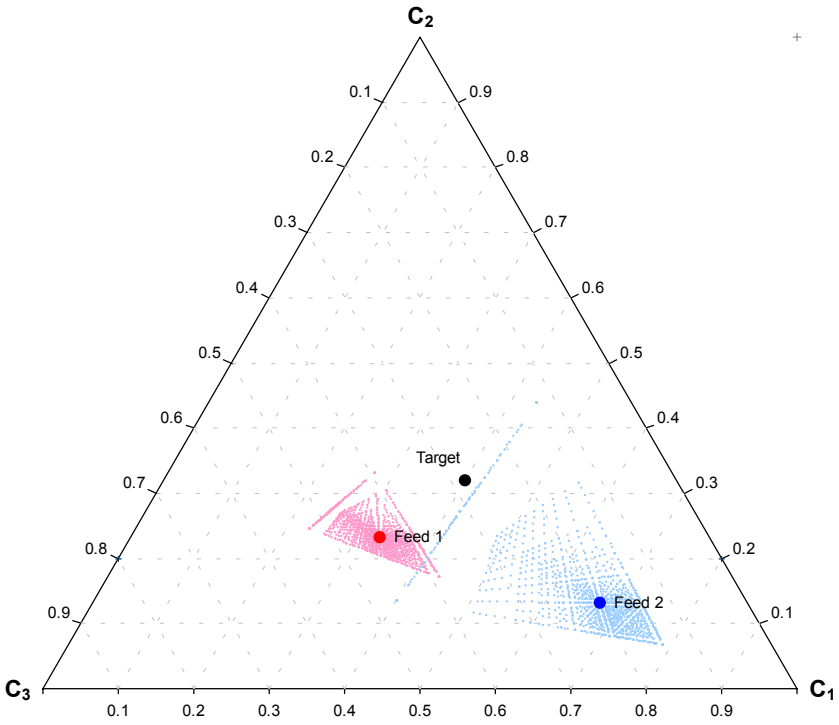

Figure 6: Source-sink mapping including feasible splitting regions

Identification of Operating Sequence

It is desired to use a minimum number of processing units, thus we decide to split feed stream 2 and mix one of the products with feed stream 1. Drawing a straight line between the cluster points for feed stream 1 and the desired product provides the operating line for the mixing operation. The stream to be mixed with feed stream 1 to match the target MUST lie on this line in such a location that the target cluster is between the two streams to be mixed. Furthermore the stream must also be within the split feasibility region of feed stream 2. In Figure 7 the solid black line represents the operating line for feasible mixing agents that match the property target. However

the only cluster points that also satisfy the feasibility constraints are designated by the orange section. In this example, we decide to split feed stream 2 in such a way that the minimum amount of feed stream 1 is used. This means that when employing lever-arm analysis at the mixing point (target point), the arm representing feed stream 1 should be minimized. Using this objective, the optimal point to be mixed with feed stream 1 is the point located just on the border of the feasibility region in Figure 7. When one of the products of a splitting operation is defined the other product will be located on a straight line from the first product and extended through the feed point. How far away from the feed point the second product is located depends on the choice of split factors. In this example any set of component split factors resulting in the first product are valid solutions.

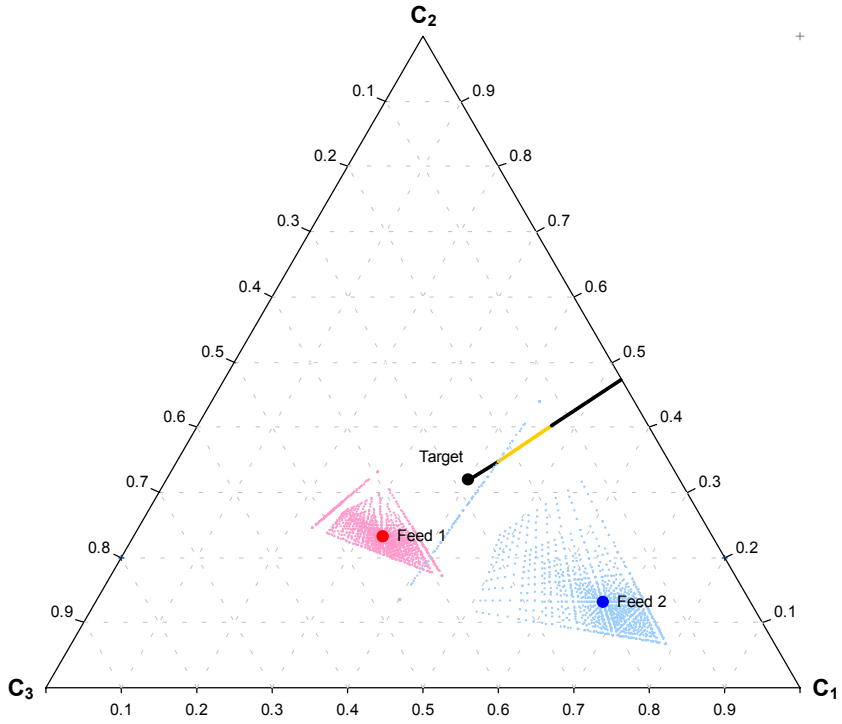

Figure 7: Feasible cluster points for mixing with feed stream 1 to achieve target

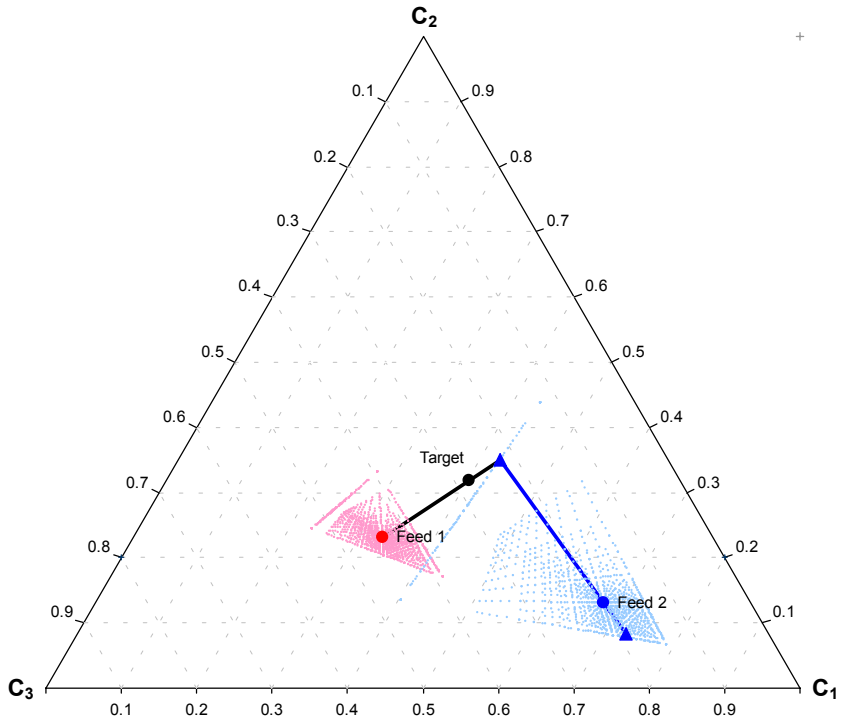

Figure 8: Source-sink mapping including feasible operational route

A powerful feature of the cluster-based source-sink mapping diagram is the ability to directly obtain the corresponding process flowsheet. This is possible because the formulation of the clusters and the unit operation models satisfy the overall balance equations. It should be emphasized that once the problem was reformulated in terms of cluster all the design calculations were performed graphically and composition free.

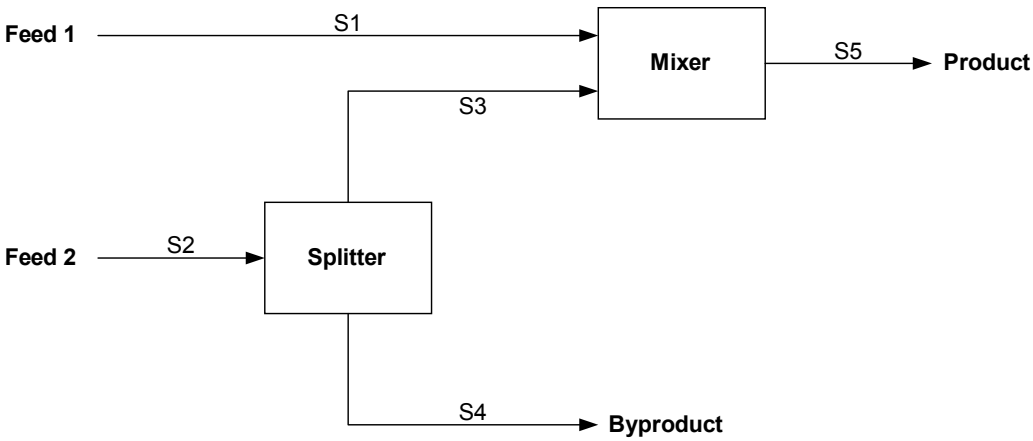

Figure 9: Feasible flowsheet obtained from source-sink mapping

Along with the process flowsheet, the stream summaries in terms of ternary cluster values and flowrates along with flowrate distributions for the two units are available. Employing the calculation sequence outlined earlier, allows for back calculating the compositions in each stream from the cluster solution. The stream summary in terms of compositions is given in Table 6.

Table 6: Stream summary using compositions

Stream ID	S1	S2	S3	S4	S5
y_1	0.1889	0.0000	0.0000	0.0000	0.0624
y_2	0.4667	0.0000	0.0000	0.0000	0.1543
y_3	0.3444	0.0000	0.0000	0.0000	0.1139
y_4	0.0000	0.1000	0.6667	0.0116	0.4463
y_5	0.0000	0.7500	0.0000	0.8670	0.0000
y_6	0.0000	0.1500	0.3333	0.1214	0.2231
Flowrate	10.0	150.0	20.25	129.75	30.25

Once again it should be pointed out that all the design calculations were performed on a composition free basis. The algorithm solves the process design problem in terms of property values providing design targets for the constitutive variables. In this particular example the design targets obtained by the reverse problem formulation are the component split factors. The second reverse problem consists of identifying the separation technique capable of matching these targets. In this contribution solution of the constitutive equations to find the matching splitting operation will not be investigated further.

CASE STUDY: VOC RECOVERY FROM METAL DEGREASING PROCESS

The metal degreasing process presented in Figure 10 uses a fresh organic solvent in the absorption column and another one in the degreaser. Currently, the off-gas VOCs evaporating from the degreasing process are simply flared, leading to economic loss and environmental pollution.

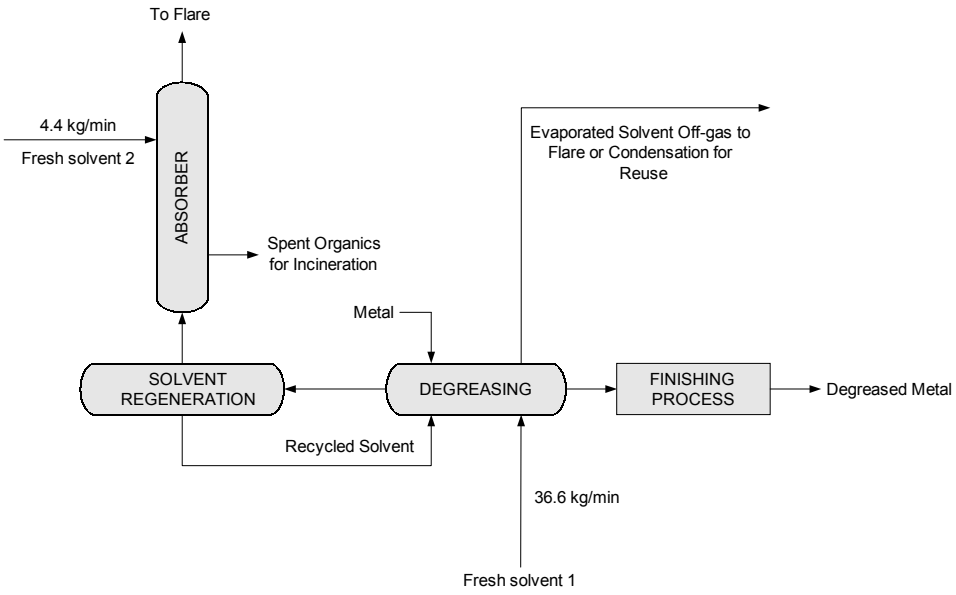

Figure 10: Original process flowsheet

In this case study the objective is to explore the possibility of condensing and reusing the off-gas VOCs, thus optimizing the usage of fresh solvents and simultaneously

identify candidate solvents for both units. Three properties are examined to determine the suitability of a given organic process fluid for use in the absorber and/or degreaser; sulfur content (for corrosion considerations), density (for hydrodynamic aspects) and Reid vapor pressure (for volatility, makeup and regeneration). The solvents to be synthesized are pure component fluids, thus the sulfur content of these streams is zero. The constraints on the inlet conditions of the feed streams to the absorber and degreaser respectively are given in Table 7, while the property operator mixing rules are given in [7].

Table 7: Sink constraints

Sink	Absorber	Degreaser
Sulfur content (weight %)	$0.0 < P_1 < 0.1$	$0.0 < P_1 < 1.0$
Density (kg/m^3)	$530 < P_2 < 610$	$555 < P_2 < 615$
Reid vapor pressure (atm)	$1.5 < P_3 < 2.5$	$2.1 < P_3 < 4.0$
Flowrate (kg/min)	$4.4 < F < 6.2$	$36.6 < F < 36.8$

Experimental data are available for the degreaser off-gas condensate. Samples of the off-gas were taken, and then condensed at various condensation temperatures ranging from 280K to 315K, providing measurements of the three properties as well as the flowrate of the condensate. These data correspond to the condensation route given in Figure 11 and Figure 12, while the sink constraints were converted to cluster values yielding the two regions for the absorber and degreaser respectively. The cluster data was plotted and the feasible mixing paths identified. Since the fresh process fluids contain no sulfur, any feasible solution will be on the C_2-C_3 axis. Lever-arm analysis is employed to identify the minimum flow solutions.

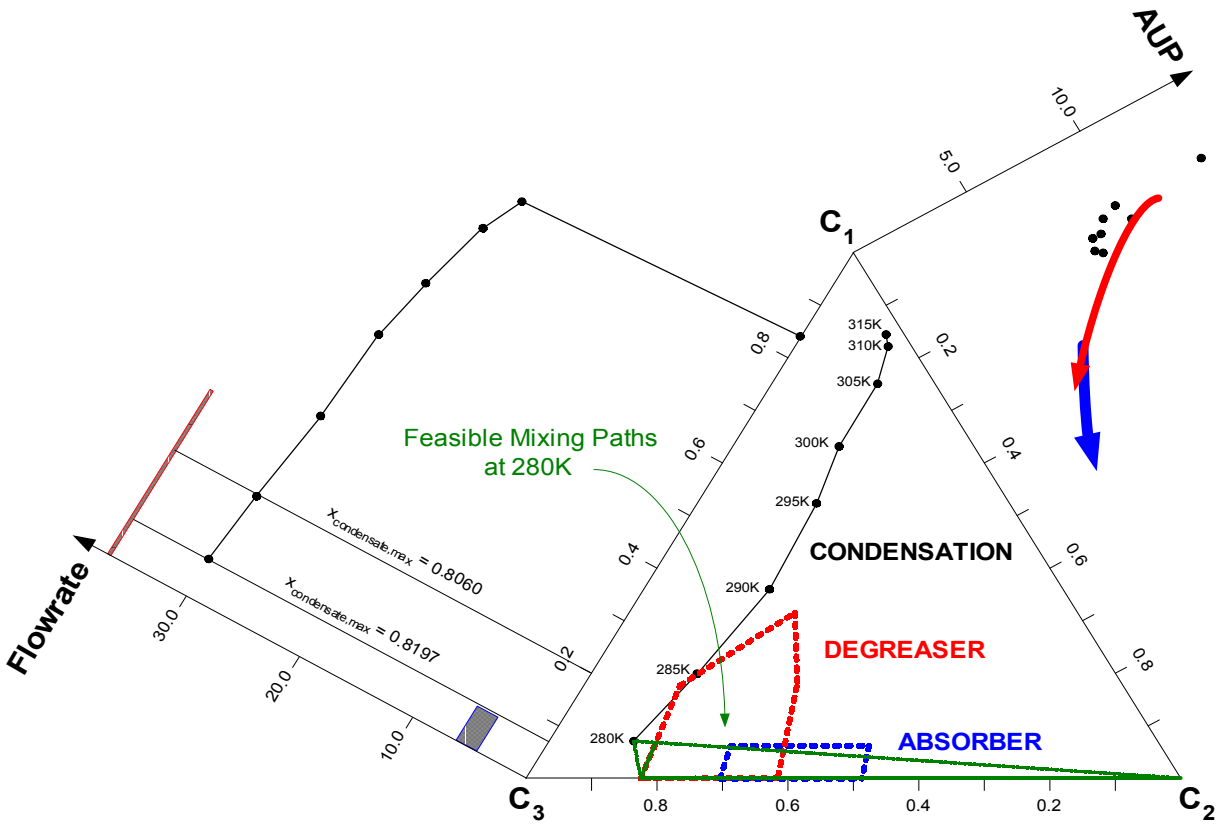

Figure 11: Source-sink mapping using condensation temperature of 280K

For a condensation temperature of 280 K (which corresponds to the highest condensate flowrate 30.0 kg/min), it turns out that the minimum feasible flowrate of the fresh is 11.8 kg/min, however the target value from the sink constraints was 6.6 kg/min, thus the same investigation was performed at 285 K. At this temperature, the condensate flowrate is slightly reduced (29.5 kg/min) however the minimum feasible flowrate corresponds to the target value of 7.1 kg/min. It should be noted that using this approach the flowrate of the fresh material has been reduced by approximately 80%. The analysis showed that the cluster solutions to the degreaser problem correspond to the degreaser points on the C_2-C_3 axis. Since all the condensate has been recycled to the degreaser, the solution for the absorber is a simple molecular design problem. Using the information obtained from the source-sink mapping analysis a computer-based tool ProCAMD [8] was invoked to synthesize candidate process fluids. Not allowing phenols, amines, amides or compounds containing silicon, sulfur or halogens, due to safety and health considerations, reduced the search space. The CAMD algorithm [9] yielded a series of candidate solvents for each of the process units. Of the candidate compounds identified by the software, iso-Pentane was chosen for the absorber and n-Butane for the degreaser.

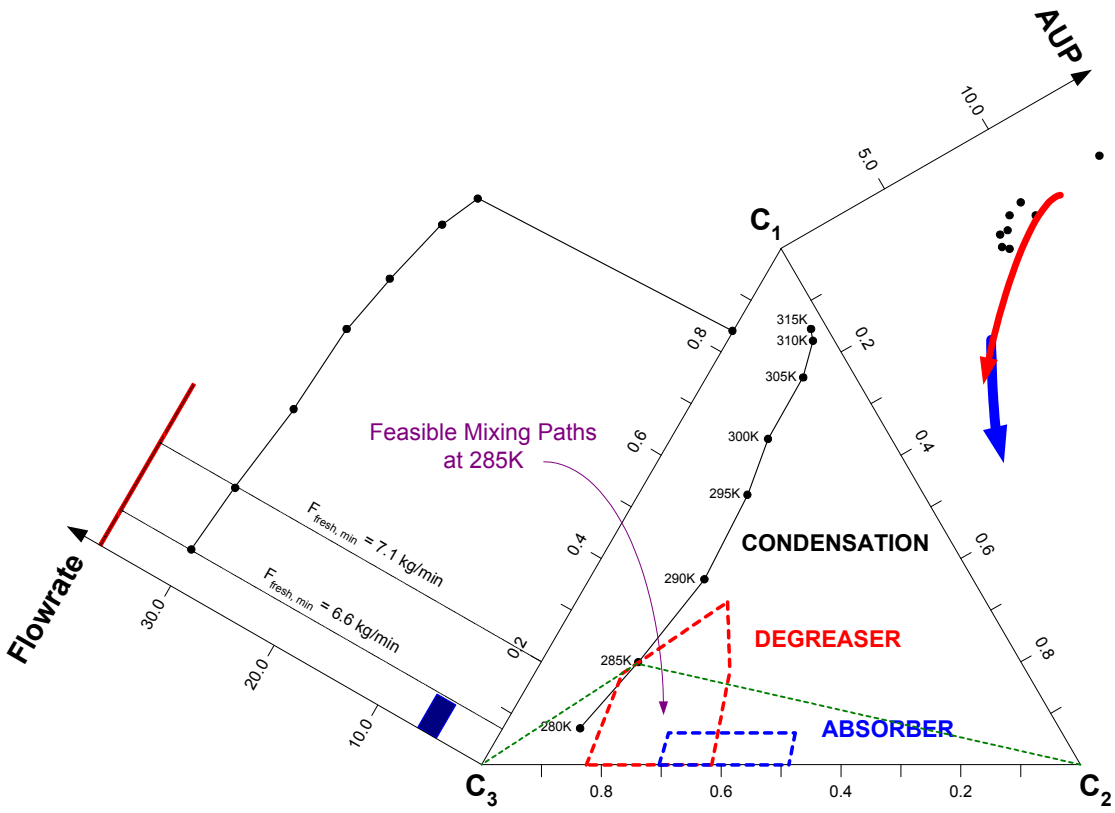

Figure 12: Source-sink mapping using condensation temperature of 285K

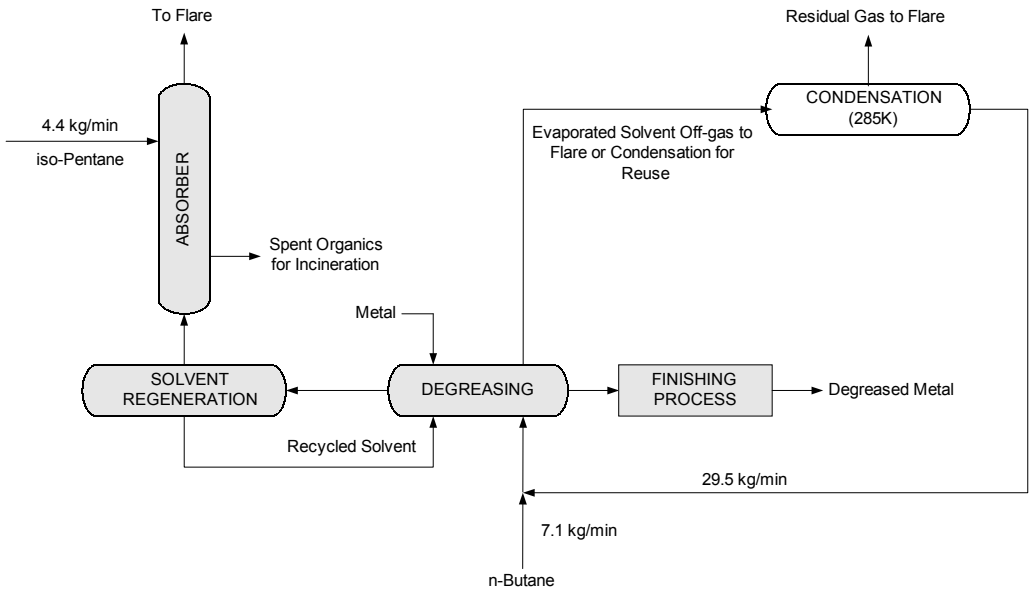

Figure 13: Revised flowsheet after property integration

It is important to point out that the case study is solved in terms of properties only, i.e. no component information or compositions were needed to obtain the design targets. The reason for this is that experimental data was available for the properties of the

individual streams. Therefore it is straightforward to convert the property values to cluster values using equations (8)–(10). The sink regions are calculated analogously to the feasibility regions for stream splitting (see Table 2); however instead of calculating cluster points for all parameter combinations of split factors, parameter combinations of the property values describing the sink constraints are used. The design calculations follow the methodology outlined previously, furthermore in terms of reverse simulation, the conditions of operation (intensive variables) for the condenser, i.e. condensation temperature, is identified, instead of the unit operation. The objective of the case study was to investigate the possibilities of using condensation of the degreaser off-gas as a substitute solvent, thus the unit operation was fixed, however the operating conditions were not known.

CONCLUSIONS

In this work, a novel framework for solving process and product design problems has been introduced. The methodology is based on reformulating the conventional forward problems into two reverse problem formulations by decoupling the constitutive equations from the balance and constraint equations. The first reverse problem is the reverse of a simulation problem, where the process model is solved in terms of the constitutive (design) variables, thus providing the design targets. The second reverse problem (reverse property prediction) solves the constitutive equations to identify unit operations, operating conditions and/or products. The main advantage of this approach is that the application range of the models has been expanded, while the problem solution has become simpler, flexible and visual. An inherent benefit of the reduction in model complexity is that the solution of the problem does not depend on the ability of the solver to handle complex process model equations. Visualization of the problem is achieved by employing recently developed property clustering techniques, which allows a high-dimensional problem to be visualized in two or three dimensions. The clusters are tailored to have the attractive features of intra-stream and inter-stream conservation, thus enabling the development of consistent additive rules along with their ternary representation. A cluster-based source-sink mapping diagram allows graphical representation of the process streams and units.

REFERENCES

1. M. R. Eden, P. M. Harper, S. B. Jørgensen, R. Gani, I. M. Glasgow and M. M. El-Halwagi (2001), Using Property Clusters for Integration of Process and Product Design, 2nd International Symposium on Process Integration, October 14-17, Halifax, Canada.

2. M. R. Eden, P. M. Harper, S. B. Jørgensen, R. Gani, I. M. Glasgow and M. M. El-Halwagi (2001), Functionality Tracking for Integration of Process and Product Design, Paper 269a, AIChE Annual Meeting, Reno, USA.

3. M. R. Eden, S. B. Jørgensen, R. Gani and M. M. El-Halwagi (2002), Property Integration – A New Approach for Simultaneous Solution of Process and Molecular Design Problems, Computer-Aided Process Engineering, 10, Elsevier (in press).

4. M. D. Shelley and M. M. El-Halwagi (2000), Component-less Design of Recovery and Allocation Systems: A Functionality-based Clustering Approach, Computers and Chemical Engineering, 24, 2081-2091.

5. B. M. Russel, J. P. Henriksen, S. B. Jørgensen and R. Gani (2002), Integration of Design and Control through Model Analysis, Computers and Chemical Engineering, 25, (in press).

6. M. M. El-Halwagi (1997), Pollution Prevention through Process Integration: Systematic Design Tools, Academic Press.

7. G. Parthasarathy and M. M. El-Halwagi (2000), Optimum Mass Integration Strategies for Condensation and Allocation of Multi-component Volatile Organic Compounds, Chemical Engineering Science, 55, pp. 881-895.

8. CAPEC (2001), ICAS User Manual, Department of Chemical Engineering, Technical University of Denmark.

9. P. M. Harper (2000), A Multi-Phase, Multi-Level Framework for Computer Aided Molecular Design, Ph.D. Thesis, Department of Chemical Engineering, Technical University of Denmark.