Minimising environmental impact using CBR: An azeotropic distillation case study

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Abstract: This paper describes a Case Based Reasoning (CBR) system which aids the design of process sequences aimed at the separation of ternary mixtures containing azeotropes. CBR is an appropriate technique for design since it is rare that a completely new problem is encountered and thus solutions for previous problems may be adapted to suit the current situation. The system is able to store, categorise and retrieve appropriate design cases for this class of problem. Also, the system stores indexed design cases within a library. These are organised according to an existing classification system for azeotropic mixtures which enables appropriate cases to be retrieved rapidly and efficiently. Additionally, it is possible for the system to produce an abstract description of the RCM and separation process, so that the designer may more easily apply the library case to the problem in hand. This description is also the first step towards the automation of the case adaptation step. Finally case study is presented which illustrates the use of the system.

Keywords: *Case Based Reasoning, Azeotropic Distillation, Chemical Process Design.*

1. INTRODUCTION

In this paper we describe a Case Based Reasoning (CBR) system to aid the design of process sequences for the separation of ternary mixtures containing azeotropes (mixtures which cannot be separated by a single distillation column due to molecular interactions leading to non-ideal behaviour). The aim is to separate one of these mixtures by adding a third component (entrainer) and using a network of distillation columns. Design of such flowsheets has been previously described and investigated, e.g. [Doherty, 85].

While the addition of the entrainer is a requirement for the desired separation to take place, it also increases the amount of potential pollutants and, therefore, environmental damage. Work has been carried out at Edinburgh to develop methods for the determination of the process flowsheets which minimise the amount of entrainer used [Manan, 1998].

CBR [Slade, 1991][Kolodner, 1991] is a technique developed to solve problems using information from previous decisions and is an alternative solution to rule-based systems. It is typically used where it is not possible to determine rules, because, for example, the problem domain is complex and there is not enough experience or knowledge available to deduce useful rules. Instead of applying rules, the current problem is compared with previous solutions stored within a library of cases. The most similar cases are then proposed as solutions to current problem, after being adapted to the new context.

CBR has the potential to be a useful methodology in design since rarely will a completely new problem be encountered. CBR has previously been used in the field of engineering design: Maher and de Silva Garza developed systems for structural design (civil engineering) [Maher, 1996], Surma and Brauschweig used a graph based approach for indexing of process flowsheets [Surma, 1996] and Domeshek et al. have developed tools for the design of case based design aids [Domeshek, 1994]. Other work has been carried out in other fields, such as of waste water treatment plant operation using CBR for learning and adaptation [Sánchez et al., 1997] and also for process equipment selection [Kraslawski et al., 1995].

We have developed a system using a CBR to retrieve similar separation problems from a case library, with the aim of adapting these to the current separation problem. The task is not a trivial one since a series of unit operations need to be used within a flowsheet (i.e. a network of processing units) involving recycling of streams for reasons described in the following sections.

2. PROBLEM DESCRIPTION

Often within a chemical plant a desired product may be mixed with a contaminant (e.g. an unreacted feed or the product of an undesired side reaction) which must be removed in order to achieve the desired product purity. It is common, for economic reasons, to use distillation to separate them. However, certain components interact with each other forming mixtures known as azeotropes which limit the scope of separation, i.e. it is not possible to achieve a purity greater than that of the azeotrope via standard distillation. For this reason, a third component known as an entrainer is added to the mixture to enable further separation. An example of an azeotropic mixture is the one formed by isopropyl alcohol (IPA) and toluene. Acetone is an example of an entrainer which can break the azeotrope. The process aim is to separate the product from the contaminant while keeping the entrainer within the process by means of recycle streams.

By adding an entrainer new molecular interactions are introduced and these are represented on a diagram known as a residue curve map (RCM). Every point inside the RCM represents a mixture of three components with fixed compositions. Such diagrams show important physical properties (see Figure 1):

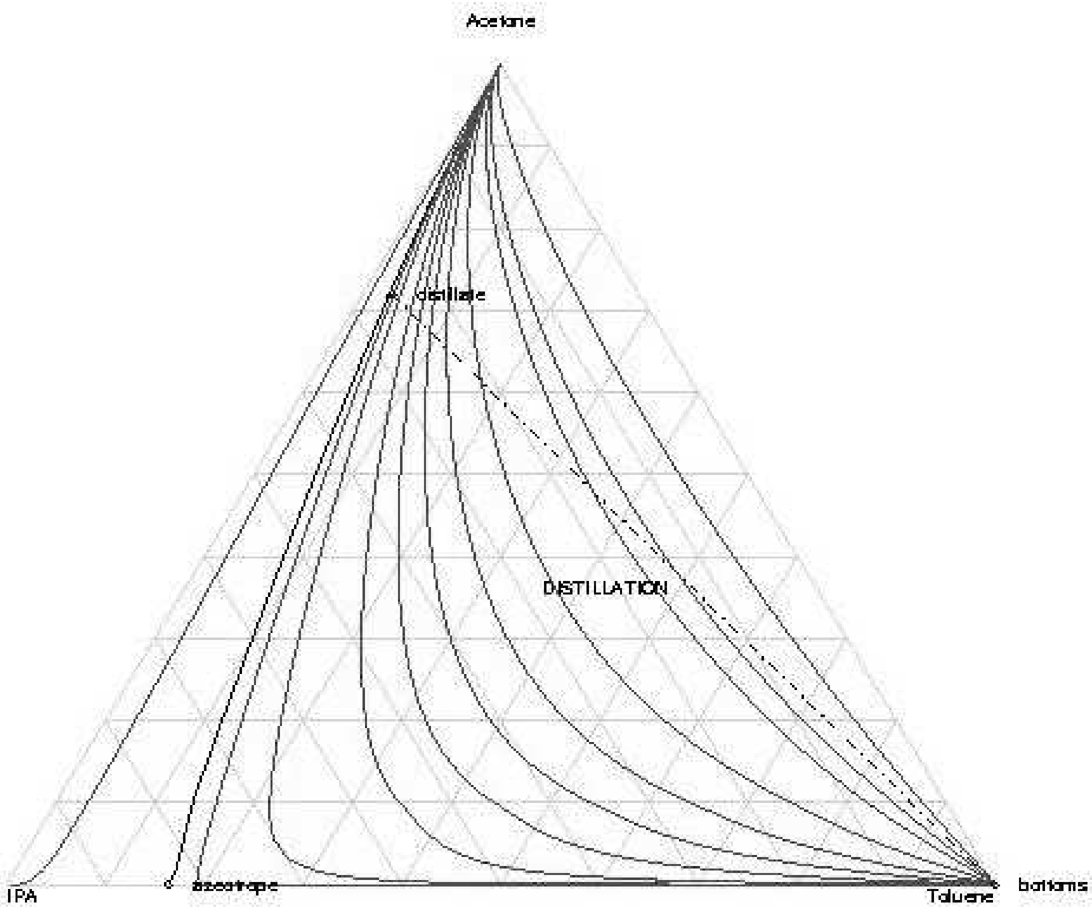

Figure 1 : Residue curve Map for the system of Acetone, Isopropyl Alcohol (IPA) and Toluene

- *pure components*, the three vertices of the RCM, e.g. **`Acetone, IPA`** and **`Toluene`**. By convention pure components are ordered counterclock-wise in increasing order of volatility starting with the low boiling component at the top of the RCM.

- *azeotropes*, binary (formed by two components) and ternary (formed by three components), e.g. the point between **`IPA`** and **`Toluene`** is a binary azeotrope.

- *residue curves*, representing the trace of compositions produced by simple batch distillation of an initial ternary mixture, e.g. the curved lines going from **`Acetone`** to **`Toluene`** or **`Acetone`** to **`IPA`**. The two products obtained from a distillation column must lie on the same residue curve.

- *distillation boundaries*, arise from the curvature of residue curves and the location of ternary and binary azeotropes, see for example the line going from **`Acetone`** to the **`azeotrope`** . It is not possible to cross straight distillation boundaries using distillation, i.e. it is impossible to separate a mixture into two other mixtures in different distillation regions. Curved distillation boundaries can only be crossed under certain conditions.

However, two streams on either side of a boundary may be mixed giving a mixture on either side of the boundary (depending on the relative amounts of each of the original streams). Thus, by distilling and mixing streams it is possible to separate mixtures across distillation boundaries and past azeotropes.

Additionally, process units can be represented in an RCM as straight lines, e.g. the **`DISTILLATION`** column separating the **`feed`** into **`distillate`** and **`bottoms`** streams in Figure 1.

Construction of a flowsheet to fulfill a process objective may not be a simple task. It requires the selection of a number of distillation columns and mixers and their connectivity, and a decision on the intermediate streams composition, see Figure 4 for an example of a flowsheet. Furthermore, it is possible that there may be more than one solution. Then it is important that the best solution in terms of various factors (including environmental impact) is selected. CBR may help the designer by either retrieving an appropriate similar case from a library or by adapting one to create a new solution. This new solution may then be stored within the case library. However, in order to do this, there must be a number of indices available. Firstly, it must be possible to categorise RCMs with similar features, e.g., number of azeotropes and distillation regions. Secondly, the CBR system must be able to find a process with similar goals and performance. Once this information has been retrieved from the case library it is then possible for either the designer or the CBR system to adapt the case for the current problem.

3. REPRESENTATION

Currently the CBR system is able to store a number of library case solutions. This representation of library cases includes a description of the physical data, i.e. the components, azeotropes, distillation boundaries and regions. Individual residue curves are not represented. Additionally, the system is able to record for each instance of RCM a number of different alternative separation processes. Each process consists of a number of process units (mixers and distillation columns) and their connectivity. Lastly, the objectives and performance of a separation process are represented by the existing feed and desired product points. A separation process retrieved from the case library is described in an abstract manner assisting the adaptation of the process case to a new problem. These features are described in more detail in the following sections.

3.1. Indexing

In order to enable retrieval of library cases the CBR system is able to determine a characteristic index for the component data and the process objectives and performance (the feed and product points) within the RCMs.

A very large number of azeotropic systems have been experimentally recorded. We have adopted the RCM classification developed by Matasuyama and Nishimura [Matsuyama, 1977] which takes into account the number and type of azeotropes (i.e. whether they are binary or ternary, and whether they are maximum, minimum or intermediate boiling azeotropes). One hundred and thirteen different classes of RCM have been identified. For example, an RCM may be given the classification **0–2–0** (see Figure 1) meaning it has one minimum boiling binary azeotrope which is between the intermediate and high boiling components and no ternary azeotropes.

Process objectives and performance are indexed by describing the positions of the process feed and the products. The positions are given in terms of the distillation region and whether it is a pure or near pure component. In turn, each distillation region may be described in terms of the pure components and azeotropes which are the intersections of the boundaries of the region. In order to compare RCMs of different mixtures, pure components are described in an abstract manner as the low, medium or high boiling component. It is common that products are pure or near pure components whereas the feed consists of a mixture of two or three components.

A qualitative description of the process may also be made, i.e. the process units, such as distillation columns and mixers, are described in terms of their relative position within the RCM.

Thus these features enable the system to:

- retrieve RCMs for similar mixtures from a library of cases
- for these RCMs determine whether there are any processes with analogous objectives and performance (feeds and products).
- produce an abstract or qualitative description of the process to aid the designer in the construction of a new process and as a first step to the automatic adaptation for the current problem.

4. IMPLEMENTATION DETAILS

This system is programmed in CommonLisp and uses the GARNET [Garnet, 1993] toolkit for its object system and graphical interface.

4.1 Physical data representation

Each RCM is stored as a GARNET object which consists of other objects :

- pure components with their boiling points and names.
- azeotropes and their boiling points and compositions (i.e. their positions on the RCM).
- distillation regions, which are stored as a series of triangles (garnet-objects). The vertices of the triangles are either azeotropes, pure components or `auxiliary' points which allow curved distillation boundaries to be represented.

4.2. Process representation

Each process is represented as a series of processing unit objects (mixers and distillation columns). Each mixer or distillation column is defined in terms of three process points: for a mixer two inputs and an output and for a distillation column one input and two outputs. When processing units are connected by streams (the output of one unit is the input of another), each point (and thus the process unit) contains information on what (if any) other point it is connected to, thus enabling the process network to be recorded.

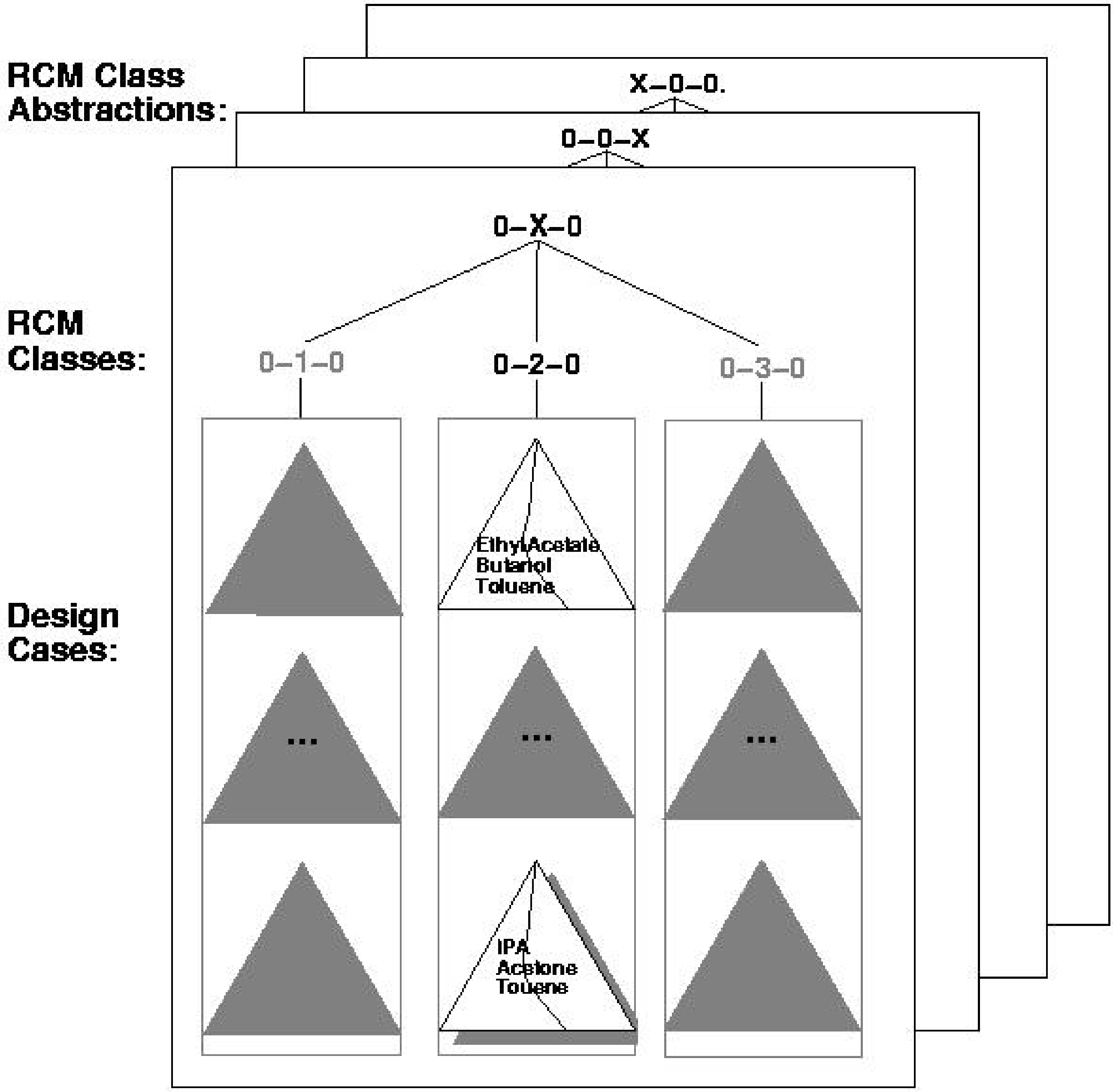

Figure 2: The case library is organised according RCM classes and their abstractions.

4.3 Case library

The case library is organised as a tree, whose structure is shown in Figure 2. Each generic group of system classifications, or RCM class abstractions (for example **0-X-0** which, represents all classes which have only one binary azeotrope between the intermediate and high boiling components), has a series of RCM classes, which conform to that particular abstraction. For each class a list of physical systems (i.e. the physical data comprising the RCMs) is stored which in the library is shown in Figure 2. For each of these cases one or more process flowsheets may be associated. For example in Figure 2 there are two processes for the system: `IPA–Acetone–Toluene`, which is of class `0–2–0.` The two cases differ in respect of the feed position, i.e. which distillation region the feed is in. Storing these two processes with different feed positions enable a greater range of problems to be solved and the library to be more compact since two processes are associated with one RCM. By storing the cases within the library in a systematic manner appropriate cases may be retrieved more efficiently since once the RCM class abstraction of the design problem has been determined only those cases (i.e. RCMs and process flowsheets) of that class abstraction need be searched and tested.

5. A CASE STUDY

In this section we discuss the design of a separation process for a mixture of acetone (medium boiling entrainer), isopropyl-alcohol (IPA) and toluene into pure IPA and toluene. The entrainer is to be recycled within the process. The RCM is shown in Figure 1 and the data recorded within the CBR system is shown in Figure 3. Note that, one azeotrope and two distillation regions are present. Here the objective points are IPA and toluene, i.e. the bottom left and right hand vertices of the RCM, since it is desired to produce pure IPA and toluene.

Although it is feasible to separate an IPA/toluene mixture using only two distillation columns, a very large amount of entrainer is required due to the distillation boundary pinch point approaching the entrainer tip [Manan, 1998], as shown in Figure 1. A preconcentrator column (**P-1** or **P-2**) decreases the entrainer flowrate needed. Figure 4 shows the two different processes found by applying the entrainer minimisation techniques proposed in [Manan, 1998]. They correspond to either one of the possible binary feeds to the column: an IPA-rich feed (left of the azeotrope, Figure 3(a)), or a toluene-rich feed (right of the azeotrope, Figure 3(b)).

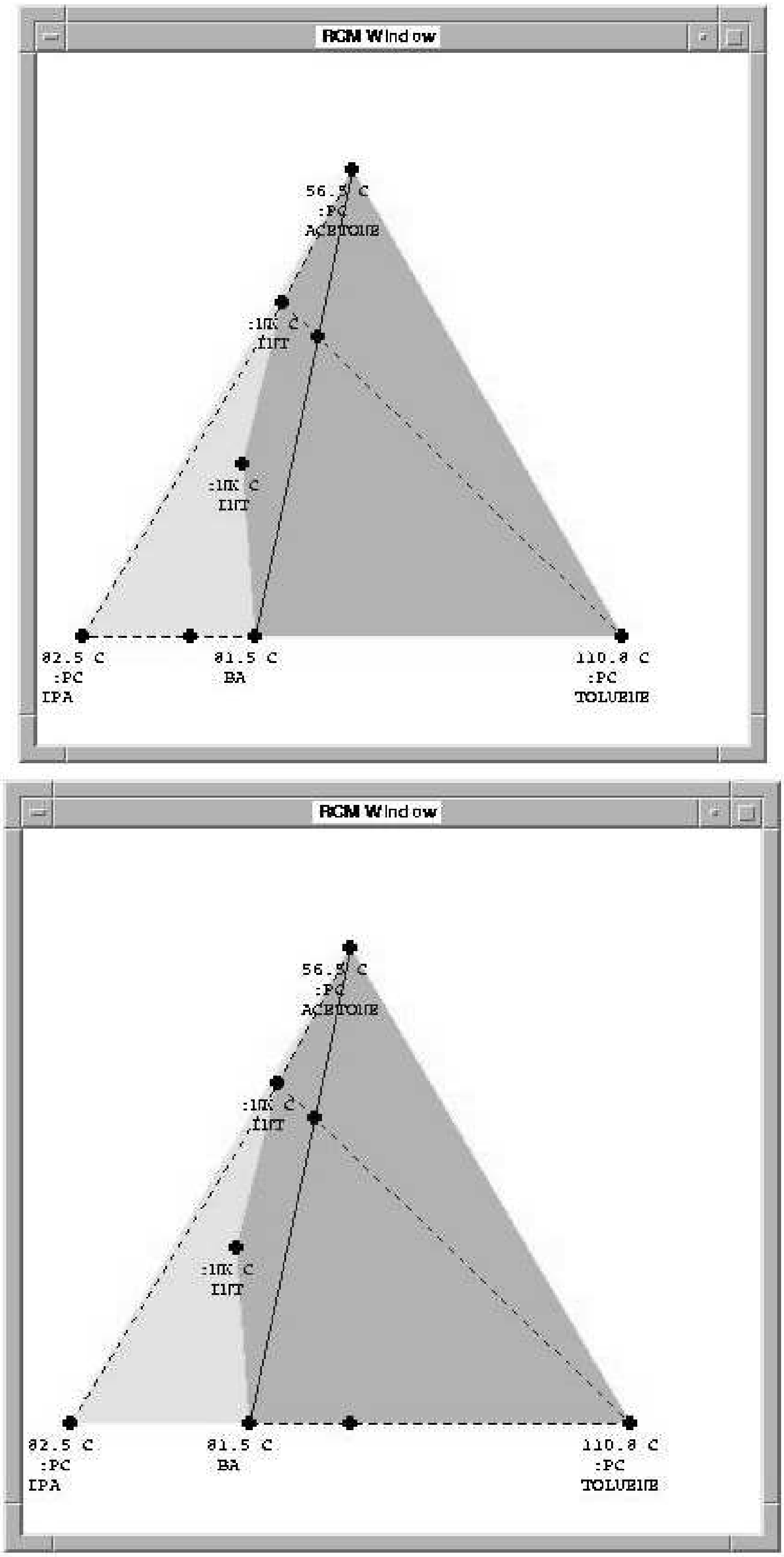

Figure 3: The two proposed processes for the Acetone-IPA-Toluene system.
Dotted lines represent distillation columns whereas solid lines are mixers.

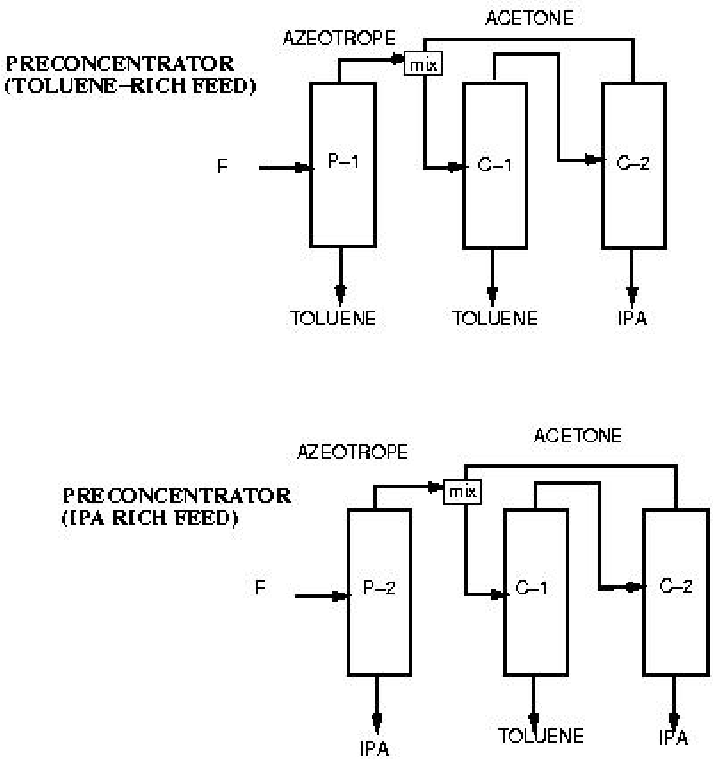

Figure 4: Proposed solutions for the system of Acetone, Isopropyl Alcohol and Toluene.

By storing the solutions in Figure 4 it is possible to ensure that a designer faced with a similar problem will be advised with the best solution in environmental terms.

5.1. Indexing

In this section a similar design problem is analysed (i.e. one with different components but with an RCM of the same class and similar process objectives) thus showing how a CBR system may be used to its best advantage. The example system consists of Ethyl Acetate, Butanol and Toluene (see Figure 5).

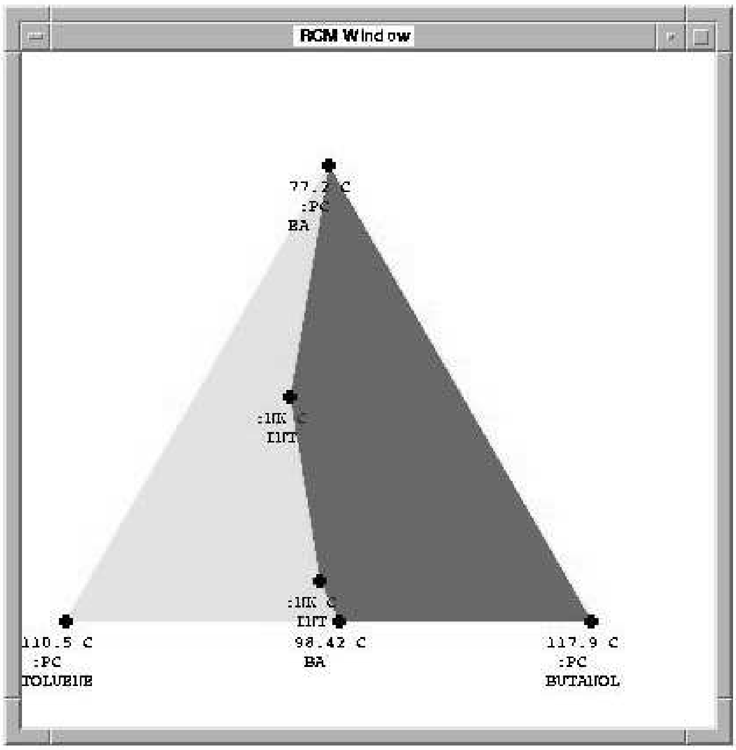

Figure 5: The RCM for the Toluene – Butanol – Ethyl Acetate (EA) system..

Since both systems i.e., Ethyl Acetate-Butanol-Toluene, and IPA-Acetone-Toluene are of a same class, i.e. **0–2–0**, an illustration of how the system will work may be given.

Two solutions are stored within the case library for the IPA-Acetone-Toluene system, which are indexed as discussed earlier depending on the position of the feed, and the objectives.

The CBR system is able to determine the positions of the objectives and feeds in an abstract manner (e.g. that the feed, or any other point, is either in the low-medium-binary-azeotrope region or the high-low-binary-azeotrope region in this example). Using this description the system is able to determine whether for any of the RCMs in the case library there exists a process which matches the current process objectives.

For example, if it desired to separate a mixture of ethyl acetate, butanol and toluene into pure butanol and toluene, starting with a feed in the butanol-binary azeotrope-ethyl acetate region, then the CBR system will determine that the performance and objective points are as follows:

- objective point 1 - (toluene) in region low-medium-binary azeotrope,
- objective point 2 - (butanol) in region high-low-binary azeotrope, and

- feed point - in region low-medium-binary azeotrope,

Thus, the lower solution shown in Figure 4 will be retrieved as a possible indication of how the solution may be constructed. To help with construction of the new process and as a first step towards automation, an abstract description of the process is be generated. It includes a description of the process units, how they are connected, which regions they are in, and a description of the process objective and feed points. For example, the lower process in Figure 4, i.e. the process for toluene rich feed, has objectives and feeds which may be described as follows.

- **FEED - LOW-HIGH-BINARY-AZEOTROPE**
- **OBJECTIVE 1 - LOW-MEDIUM-BINARY-AZEOTROPE**
- **OBJECTIVE 2 - HIGH-LOW-BINARY-AZEOTROPE**

Additionally the first unit may be described in an abstract manner as follows:

```
PROCESS UNITS:

• P-1:
     FEED :feed
     TOPS :BA          :connected [MIX-1 :feed1]
     BOTTOMS :PC-HIGH  :connected nil
  Touches :axis-LOW-HIGH :region HIGH-BINARY-AZEOTROPE-MEDIUM
```

This information assists the designer with the construction of a new similar process for the current problem on the new RCM. For example, the designer can see that the preconcentator unit P-1 should in the new system of ethyl acetate-butanol-toluene again lie on the axis between the highest boiling component and the binary azeotrope, i.e. butanol and the binary azeotrope.

6. FUTURE WORK

To enable a full CBR system it is necessary to complete the case adaptation stage by applying the qualitative description of the process to the context of the new RCM. Future work will include this as well as the storing of the new adapted design in the case library providing it meets with the designer's approval.

7. CONCLUSIONS

In this paper its has been illustrated how a Case Based Reasoning system may be used to retrieve similar designs from a library and use these to prompt the designer with the most appropriate design for azeotropic distillation. By storing environmentally sound designs within the case library we ensure that the designer minimises any environmental impact.

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