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Design acceleration in chemical engineering

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Abstract

Nowadays, chemical engineering has to face a new industrial context with, for example, the gradually falling of hydrocarbon reserves after 2020–2030, relocation, emerging of new domains of application (nano-micro technologies) which necessitate new solutions and knowledges ... All these tendencies and demands accelerate the need of tool for design and innovation (technically, technologically). In this context, this paper presents a tool to accelerate innovative preliminary design. This model is based on the synergy between: TRIZ (Russian acronym for Theory of Inventive Problem Solving) and Case Based Reasoning (CBR). The proposed model offers a structure to solve problem, and also to store and make available past experiences in problems solving. A tool dedicated to chemical engineering problems, is created on this model and a simple example is treated to explain the possibilities of this tool.

Keywords: Innovation; Design; Case based reasoning; TRIZ; Chemical process

1. Introduction

Nowadays, engineers have to design and solve problems with different degree of difficulties. Sometimes, these activities are easily done with the use of tables, correlations, models ... On the other hand, some problems are very complex and the resolution necessitates a strong mobilization of time and resources. Within this framework, companies mobilize their resources in order to improve their products and processes or to create new ones, to ensure their future. The rapid changes of their surrounding world (economic, new environmental constraints, reduce time to market ...) impose new challenges to the companies. Chemical engineering industries do not escape from this context; moreover, they also have to anticipate some problem, like the gradually falling of hydrocarbon reserves ... In this context, the acceleration of the processes of innovative conception is a crucial question, where two fundamental elements interact: knowledge and creativity.

Knowledge capitalization comes from Artificial Intelligence, and consists in the reuse of past experiences which are acquired, deployed and checked during problems solving, in a specific domain. Several methods are available to store and reuse past experiences. But in the context of this study, Case Based Reasoning (CBR) is the most interesting one, because of its affinity with human learning and its effectiveness proved in chemical engineering.

The principal drawback of this kind of methods appears when you have to innovate: an innovative solution cannot be reached by using past experiences in one specific domain. With CBR you can innovate but most of the time, the proposed solution has a low level of innovation (incremental innovation). To propose a solution with a high level of innovation (rupture innovation), generally you have to use new knowledge (coming from others technical domains for example). To avoid this drawback, the theory TRIZ (Russian acronym for Theory of Inventive Problem Solving) can be used. This theory which refuses compromise in its process of problem solving, was built on the ideas that it exists universal ways to solve problems and that every engineers can propose innovative solutions. TRIZ is based on a scientific step, and proposes several tools which allow the generation of innovative ideas and facilitate the design of new processes (whatever the technological field is). This theory only starts to appear in chemical engineering research [1,2], but it is used by several companies in the domain.

The aim of this paper is to propose a synergy between CBR and TRIZ and to develop a tool based on the model of this syn-

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ergy in order to accelerate conception in chemical engineering. Moreover, Srinivasan and Kraslawski [1] in their conclusion underline the need of that kind of tools. The goal of that tool is that every engineer can propose rapidly a solution when he faces a new design problem.

The two next sections of this article present both element of the synergy: CBR for the second section and TRIZ for the third one. These two sections are followed by the presentation of the model of the synergy. And before concluding, an example of all the possibilities of the tool is presented with a mere unit operation: the Simulated Moving Bed.

2. Case Based Reasoning (CBR)

2.1. Presentation

Case Based Reasoning is a useful methodology for initial steps in design. CBR methodology came from Schank [3] research on human memory and dynamic memory. This resulting methodology has proved its efficiency in a wide range of applications. One reason for this wide application of CBR is due to its most important advantage: its affinity with human learning. CBR is a memory based methodology, thus reflecting human use of remembered problems and solutions as a starting point for a new problem solving. The general principle applied in CBR is: similar problems have similar solutions. Consequently, CBR is a methodology for problem solving based on past experiences. CBR tries to solve a new problem by retrieving and adapting known solutions of similar problems.

The central notion of this methodology is a case, which corresponds to the problem description, its solution and eventually some comments. A case is a contextualised piece of knowledge representing an experience. Many cases are gathered and stored in a memory, named the case base. Consequently, this case base is composed of two spaces as illustrated in Fig. 1: the problem space and the solution one. For solving a problem with CBR, you have to describe it, then measured the similarity of this input problem (target problem) with problems stored in the case base and retrieved the (or more than one) most similar problem and its solution. The next step is to reuse the retrieved solution for the target problem and to make a revision of the proposed solution, if necessary. Finally, the input problem and its solution form a new case, which is stored in the memory in order to increase its



Solution Space

Fig. 1. Case base representation.



Fig. 2. CBR cycle.

effectiveness for problem solving. These are the general steps of the CBR cycle, they are detailed in the next part.

2.2. CBR cycle

The individual steps in the CBR methodology form a cycle, referred as the R⁴ model: Retrieve, Reuse, Revise and Retain [4], Fig. 2. But before using the CBR cycle, a preliminary important step consists in representing the experiences contained in the cases for reasoning purpose. There is a wide variety of representation formalism for cases, but only three main categories could be extracted [5]. The feature-vector representation is the more appropriated to the purpose of this article. This approach represents a case as a vector of feature-value pairs, for the problem and solution descriptions. Of course, problems and solutions are described with different numbers of features and different informations. After this preliminary step, the CBR cycle can be started:

- 1. *Retrieve*: According to a new target problem, this step of the CBR cycle is the retrieval from the case base, of previous cases that are similar. Here, the central issue is the similarity measurement in order to find the most useful case to solve the target problem. The similarity between two cases is measured by a function which depends on the type of features value: words, numerical values, diagrams, plans ...
- 2. *Reuse*: The goal of this step is to propose a solution to the target problem, derived from the solution(s) of the retrieved case(s). This solution is used as a starting point for the problem resolution. Reusing previous cases solutions can be as trivial as applying the solution without modification (for example when the retrieved case is sufficiently similar). However most of the time, there is a gap between the target and similar problems, then the retrieved solution does not exactly correspond to the target problem and it often needs an adaptation. This adaptation becomes complex when the differences between the both problems are important.
- 3. *Revise*: The previous adapted solution is used as the starting point for the target problem resolution. Even after the reuse step, the solution perhaps needs some adjustments to

fit the target problem. Consequently, the user revises the solution generated in the previous step to resolve the discrepancy between the desired and the adapted solution: by simulation, optimization, for example.

4. *Retain*: After its resolution, the target problem and its associated solution form a new case. If it brings something, the CBR system may learn this new case by its incorporation into the case base. This step extends the cover of space problems, increasing the CBR effectiveness by enlarging experiences retrained. In this paper we simply store the new problem description and its associated solution but more information concerning this new case and its resolution can be added and recorded too (for example: failed tries before to reach the solution, comments on the implementation of the solution).

This interesting methodology is used in numerous domains: medicine, chemical, design ... CBR systems have recently proved their effectiveness in chemical engineering with applications in: process conception [6], process separation [7], selection of internals for reactive distillation [8,9], selection of mixing equipment [10], alternative representation of chemical process [11], minimising environmental impact [12]...

2.3. Conclusion

The CBR approach is very interesting for complex problems resolution because it can quickly offer a solution and accelerate design. It is based on the fact that the second time you have to solve a problem (or a part of a problem) you do it quicker and easer because you recall your success, and mistakes are avoided. CBR have undeniable advantages like: its facility of use and maintenance, the reasoning based on similar cases in the same technical domain ... However, this last advantage becomes a drawback for our objective, because with focusing only in a particular domain, solutions which appeared effective in others domains are avoided. And the diversity of domains taken in account often has a positive and favorable impact on the solution quality and innovation. In addition to this, the principal drawback of CBR system appears when the retrieve step does not find any similar cases for the target problem. In this situation, the designer must change its approach and try to find a solution with others types of methods like the theory presented in the next section.

3. TRIZ theory

3.1. Presentation

One of the methods that allow innovation to be generated in rupture is the TRIZ theory. This theory has been developed in former USSR since 1946 by Altshuller [13] and it is used in the whole technical world. TRIZ is the Russian acronym for Theory of Inventive Problem Solving.

TRIZ is a useful theory to systematize innovation and consequently to improve design for our purpose. Altshuller considers creativity as an exact science and intends to develop tools for detaching invention from human individual aptitude. Thanks to TRIZ, each engineer can generate and produce innovative ideas. Refusing the idea that innovation is a prerogative of a higher intellect or the result of a random process, Altshuller started his research with the following assumption: there are some universal principles to innovate and to solve all the problems.

This theory resulting from Altshuller and his team's work, comes from patent analysis (nowadays more than 2 millions), scientific literature analysis. All these analysis lead to several concepts and tools that compose TRIZ.

It is important to underline that TRIZ is not a miracle theory that gives in all cases innovative ideas. Its goal is to direct the solution research to a good direction thanks to analogies between technical domains.

When a new problem solving is faced, methods like brainstorming, trials and errors randomly explore the solution space, resulting in an important resolution time. TRIZ avoids this random exploration with a convergent process that delimitates the research space. This process is included in TRIZ tools, and channels the efforts to an ideal solution. This time reduction for the research of solution is interesting to accelerate design. The principle of problem resolution is illustrated in Fig. 3:

- Modelisation of the real initial problem in a generic problem (TRIZ tools are dedicated to this step).
- Use of some TRIZ resolution tools to give a generic solution to the generic problem (proposition of research directions for the solution).
- Transformation of the theoretical generic solution to a real solution adapted to the real problem.

With this principle, the problem is abstracted to a higher level and the user must let express its creativity at the last stage during adaptation stage. Traditional methods (brainstorming . . .) try to find a specific solution to the problem which is often difficult and takes a lot of time.

3.2. Tools and concepts descriptions

The TRIZ theory has numerous tools and concepts like evolution laws and an algorithm of resolution ARIZ. To have an overview of all the tools, the reader can refer to [14,15] ... In the context of this paper only tools and concepts concern by this research are presented:



Fig. 3. TRIZ problem solving process.

- Ideal Final Result: Every invention or problem resolution promotes the development and improvement of a technical system. The Ideal Final Result (IFR) is a concept that will eliminate negative effect in the system, preserving its capacity (even increase efficiency) to produce a useful effect by itself (without: human intervention, energy, new systems, cost . . .). The IFR is the ultimate goal to reach in a technical system evolution. This is a psychological concept that allows a complex problem to be solved by a mere solution. Most of the time, it gives a utopian result but it offers a way of reflexion seldom explored. During IFR reflexion, you have to imagine solutions outside technological reality: you do not matter if it is technologically possible or not to reach IFR. Furthermore, the IFR serves as criterion to choose in a set of possible solutions the best one because each problem can be solved in many different ways.
- *Contradiction*: Every problem is formulated as a contradiction, i.e. conflict in the system. The challenge of the TRIZ problem solving theory is to remove contradiction: when known requirements, needs, alternatives available to improve one aspect of the design do it at the expense of another aspect of this design (technical contradiction). These mutually exclusive needs have to be associated. Traditional problem solving methods solve the contradiction with a compromise whereas TRIZ refuses it and tries to propose a solution which satisfies the two aspects of the design. TRIZ can solve many kinds of problem but the theory is more powerful and gives value added when it is used to solve non-routine problems containing contradictions.

One of the most utilized tools in the TRIZ theory is the contradiction matrix, dedicated to solve technical contradiction. After its patent analysis, Altshuller had noted that the same fundamental problem had addressed by a number of inventions, and had been solved with the same fundamental solution in different technical domains but with implementations separated by several years. He had also concluded that technical problems are solved in 40 main different ways for the whole technical fields. There are named the 40 innovation principles (the principles are decomposed in sub principles to a better understanding and in order to increase the effectiveness of resolution).

The matrix tells you among the 40 principles which ones have been used most frequently to solve a problem that involves a particular technical contradiction. The second step of the patent analysis is to formalize the technical contradiction. By definition, it is a conflict between two parts of the system. Consequently, Altshuller modelised technical contradiction by the conflict between two parameters: one improved and the other one damaged. Finally, 39 parameters had been identified to describe the whole contradictions included in the patents (after a new patent analysis in 2003, the number of parameters was increased to 48 but the number of principles always stays at 40). A 39×39 matrix is built, on the line we find the parameter improved, and the damaged one on the column. The crossing between these two parameters isolates a cell which contains the 3 or 4 most frequently used principles in order to solve that precise contradiction (Fig. 4) (each principle is identified by a number which is reported in the cell). In the cell, the principles are classed in order of importance (statistical results of the patent analysis) from the more used. It is important to underline that the proposed principles do not give a solution but they limit the research domain by giving a way to explore before leaving the creativity to express.

In order to use the contradiction matrix when a new problem is encountered, the first step is to identify the problem conflict. The second one is to translate the problem in the conflict between two among the 39 parameters, and then use the matrix to find the principles able to help you for proposing a solution. To illustrate the use of the contradiction matrix, the example of the sweet pepper canning method, coming from [16], is presented.

		Damaged Parameter									
		1	2	3	4	5	6	7	8	9	10
Improved Parameter	1			15, 8 19, 34		29, 17 38, 34		29, 2 40, 28		2, 8, 15, 38	8, 10, 18, 37
	2				10, 1, 29, 35		35, 30, 13, 2		5, 35, 14, 2		8, 10, 19, 35
	3	8, 15, 29, 34				15, 17, 4		7, 17, 4, 35		13, 4, 8	17, 10, 4
	4		35, 28, 40, 29				17, 7, 10, 40		35, 8, 2,14		28, 10
	5	2, 17, 29, 4		14, 15, 18, 4				$\left(\begin{array}{c} 7, 14, \\ 17, 4 \end{array}\right)$		29, 30, 4, 34	19, 30, 35, 2
	6		30, 2, 14, 18		26, 7, 9, 39			\checkmark			1, 18, 35, 36
	7	2, 26, 29, 40		1, 7, 4, 35		1, 7, 4, 17				29, 4, 38, 34	15, 35, 36, 37
	8		35, 10, 19, 14	19, 14	35, 8, 2, 14						2, 18, 37
	9	2, 28, 13, 38		13, 14, 8		29, 30, 34		7, 29, 4			13, 28, 15, 19
	10	8, 1, 37, 18	18, 13, 1, 28	17, 19, 9, 36	28, 10	19, 10, 15	1, 18, 36, 37	15, 9, 12, 37	2, 36, 18, 37	13, 28, 15, 12	
				,				Pr	inciples	s to use	

Fig. 4. Piece of the contradiction matrix.

3.3. Example of use of the contradiction matrix

Before canning sweet pepper, the stalk and the seeds must be removed from the pod. This operation was done manually, because automation is difficult due to non-uniform shape or size of the pods. The goal is to facilitate the extraction of the stalk and seed from the pod without reducing the process productivity. The identification of the two parameters in conflict gives: parameter 32 named 'Ease of manufacture' as improved parameter versus parameter 26, 'Quantity of substance' as the damaged one. The crossing cell contains 4 principles in the following order: 35 'Parameter changes', 23 'Feedback', 1 'Segmentation', 24 'Intermediary', [14] give a precise description of all the principle and [17,18] illustrate the principles with example in chemical engineering. The parameter 35 suggests to change an object's physical state, or to change the concentration, temperature, pressure ... With this way of solution research the following innovative method can be found: the pods are put in an airtight tank (Fig. 5) the pressure is gradually increased to 8 atm. The pods shrink, and consequently there is a fracture at the weakest point: the junction between the pod and its stalk. Air penetrated the pepper until pressure equality (inside and outside the pepper). The pressure inside the tank is quickly reduced, resulting in the bursting of the pod and an ejection of the seeds, because a new pressure equilibrium is reached (inside and outside the pepper).

3.4. Conclusion

Altshuller had built TRIZ tools with a scientific analyze (patents, physical effects, chemical effects, geometrical effects, scientific literature ...) of the whole technical domains, eliminating the barriers between these different domains. With this advantage, you can beneficiate of solutions or ways of solution that had proved their effectiveness and consequently accelerate the design and also propose more innovative solutions. For each new problem solving faced, the TRIZ theory can always propose a way of solution which is another advantage. Nevertheless, for our purpose two main drawbacks had been identified: on one hand, for each new problem the whole algorithm and resolution process have to be redeployed, on the other hand TRIZ theory is difficult to use and understand without practice. This last point is partially avoided in the model presented, because the synergy proposed, in the next section, used concepts and tools that are the easier to understand (contradiction matrix presented above). TRIZ is widely used in several technical domains and in a huge number of companies, but TRIZ only starts to appear in chemical engineering research [1,2,19,20]. Nevertheless, some chemical



Fig. 5. Sweet pepper solution [16].

engineering companies used it to solve their problems, because it gives a structured method that offers a new approach to tackle problems.

4. Synergy TRIZ-CBR

4.1. Presentation

Because of the complementarities of the two approaches (detailed in [21]), it is interesting to couple both of them in order to propose a tool to support and accelerate design. This tool must offer systematically a way of solution for each new problem encountered. In this synergy, TRIZ brings the initial structure, i.e. the contradiction matrix, to produce a support to index and store cases and to propose a solution if no similar cases are found. The contradiction matrix has two roles: its initial one coupled with the case base one (avoiding the creation of a specific tool). On the other hand, CBR brings techniques to accelerate problem research and comparison with others one solved before. In traditional CBR, the central notion is a case composed of three elements: problem, solution and some comments;

Case (PB, Sol(PB), Co)

In the synergy a case is represented in the same way. For the problem description, the feature-vector representation is used. The problem must be formulated by its contradiction, because the contradiction matrix is the support of the case base. Consequently, the two first features are the contradiction parameters. These parameters are also useful to index the case base and consequently accelerate the research of similar problems during retrieval (detailed in the next part). Of course, these two parameters are not enough to describe correctly the problem, so additional features are added: the unit operation where the system is located, the type of objectives, the goal to reach, the resources identified in the system ... Concerning the solution, it is formulated with feature-vector representation too. Like in the problem representation, the use of the matrix contradiction imposes some features. In the contradiction matrix, the principles give a way of resolution; consequently, a solution is represented by the principle which allows finding it. Here again, the principle is not enough to completely describe the solution, other features are added to detail the solution: temperature, pressure ...

4.2. Synergy cycle

After the case representation, the resolution process proposed in the synergy can start (Fig. 6). The model presented re-uses the five principal steps of the classical CBR, i.e. Representation, Retrieval, Reuse, Revise and Retain but some new functionalities are added to improve the effectiveness of resolution. The resolution process starts with the step of identification of the target problem: problem description, ideal final result, contradiction. On the one hand the IFR proposed a way of reflexion for the problem-solving step, and on the other hand it gives a criterion to the evaluation of the future solution. With that initial step all the features in the problem description are filled.



Fig. 6. TRIZ-CBR model for the synergy.

After case representation, the retrieval step finds the most similar cases to the target problem. During similarity calculation, the importance of features can be reflected by weights affected to each ones (1). The Nearest-Neighbor algorithm is commonly used to select the most similar cases (k-NN to retrieve the k Nearest Neighbors). Of course the retrieval model does not explore the whole case base in order to find the nearest neighbors, because this step would be time consuming. Moreover, the case base is still growing by adding new cases thanks to the retain step (for example). Commercial CBR tools, adopt a standard retrieval model where a decision tree index selects potentially relevant cases followed by a nearest neighbor algorithm search to select most similar cases. Without a decision tree index, for each case in the case base we have to calculate the local similarities, the global one and in a last step to rank all the cases. In our case, a problem is stored in the contradiction matrix case base thanks to its contradiction. Moreover in the case representation, the two first features are the parameters which identify the contradiction. Consequently, they are used as index to select relevant case in the subset of cases modelised by the same contradiction and then to reduce the research time. Some other features can be used to restrain the research domain as we are going to see in the example.

The global similarity between the target problem and problems stored in the case base is calculated by the following function:

$$SIM(T, S) = \frac{\sum_{i=1}^{n} w_i^* \sin_i(f_i^T, f_i^S)}{\sum_{i=1}^{n} w_i}$$
(1)

with *T*, target problem; *S*, source problem (in the case base); *n*, number of features; w_i , weight of the feature *i*; $sim_i(f_i^T, f_i^S)$, local similarity on the feature *i* between problems *T* and *S*.

The local similarity calculation depends on the type of the values of the features: numerical or textual ones. In our case,

two values of these local similarities are defined as:

Numerical:
$$sim_i(f_i^T, f_i^S) = 1 - \frac{\left|f_i^T - f_i^S\right|}{Int_i}$$
 (2)

Textual:
$$sim_i(f_i^T, f_i^S) = \begin{cases} 1, & \text{if } f_i^T = f_i^S \\ 0, & \text{if } f_i^T \neq f_i^S \end{cases}$$
 (3)

where Int_i is the difference between the maximum and the minimum values, calculated over all problems.

From the retrieval step, the process detailed in Fig. 6 considers two possibilities:

- A similar case is found in the case base. Then its associated solution is proposed and adapted to the target problem.
- Not enough similar case or worst, no similar one has been identified in the previous experiences stored. The system nevertheless proposes the principles associated to the target contradiction, and then the matrix finds its initial role. The proposed principles reduce the solution space, and then they are analyzed and interpreted and finally the designer creativity has to express, to propose a solution.

Whatever the possibility taken in the process, the two ways converge to the proposal of one solution. This solution is revised and modified to give a satisfactory result to the target problem. Finally, the process ends when the results of the implementation of the solution (success or eventually failure) and the strategy to reach it, are validated and then be retained to increase the case base effectiveness.

4.3. Conclusion

The principal advantage of the process is that, whatever the target problem there is a solution or in the worst case a way of solution proposed. Moreover, this synergy benefits of TRIZ and CBR advantages. For TRIZ, the interdisciplinary of the

domains allows really innovative solutions thanks to the opening on other scientific fields, the IFR gives a criterion to evaluate the solution (not present in other design methods). The problem formulation in TRIZ, i.e. the contradiction, reduces the time of the retrieval research by its structural indexation (reduction of the research domain compared to a search in the whole case base for a classical CBR). The CBR brings to the model its process for reusing past experiences coupled with its advantages: facility of use (because of its affinity with human way to learn), rapidity to produce a solution, and its ability to give a very precise solution to the target problem (pre-design of the solution after adaptation). The principal difficulty of this process is to identify the "good" contradiction, because when you face a problem there is different ways to formalize it as a contradiction. Moreover for very complex problem, it is possible to have several contradictions; in this case you have to formulate the most important one. To avoid this difficulty, TRIZ contains specific tools to help the user to correctly approach the problem and to clearly identify the main contradiction: Innovative Situation Questionnaire ... The next section presents a simple example of the model with the true moving bed problem (and its well-known solution; Simulated Moving Bed). This example was treated with a tool created from the model implementation. As we have seen, the model is very general but the effectiveness of the tool depends on the case base, more precisely, of its cover of the problem space. Here, the case base is filled with numerous problems especially dedicated to chemical engineering.

5. Example

The goal of this part is to highlight the possibilities of the synergy TRIZ-CBR in a mere chemical engineering example. Chromatographic separations are unit operation techniques to continuously separate a multi component mixture. This technique has recently received a new interest from researcher [22,23] because of its new applications in areas such as: biotechnology, pharmaceutical, fine chemistry ...

One of the possible technological starting points of this unit separation is the true moving bed (TMB), for which a simplified version is illustrated in Fig. 7. For the TMB separation technique, the component mixture is sent in a column where the liquid and solid phases flow in counter current directions. The liquid outlet of zone 4 is recycled to the zone 1 inlet, and conversely for the solid: the zone 1 outlet is recycled to the inlet of zone 4. Moreover, this apparatus has one feed (with the mixture to separate) and two outlets to withdraw products: extract (rich in the component the more retained, preferentially in the solid phase) and raffinate (rich in the less retained component, preferentially in the liquid phase). The main disadvantage of this technique is the flow of the solid phase, which is a complex task.

With the help of TRIZ tools (like Innovative Situation Questionnaire), the first step is to identify and formulate the drawback by the way of a technical contradiction. In this case, the contradiction can be formulated in the following way: "eliminate the solid flow without reduce the separation effectiveness and increase the operating cost". After the contradiction identifi-



Fig. 7. True moving bed.

cation, the next stage consists in the identification of the two parameters (among 39) in conflict to formulate the contradiction in TRIZ way (and of course to inform the others features):

- *Improved parameter*: the flow of the solid phase implies a difficulty of use, consequently the parameter 33, '*Convenience of use*' is chosen.
- Damaged parameter: it is the parameter 19, '*Energy spent by a moving object*'.

After the problem description, there are the two possibilities. We are going to explore both of them on the same example.

5.1. First possibility: no similar case

With this example, if we imagine that with the previous information the research in the matrix case base does not give any similar case (which is not actually the case as we are going to see in the second possibility, but the goal is to exemplify the two possibilities in the retrieval step). In these conditions, the contradiction matrix finds its initial use and gives ways of resolution with the principles. The crossing of line 33 and column 19 isolates a matrix cell with the following principle: 1 'Segmentation', 13 'Inversion', and 24 'Intermediary'. The principle 1 recommends to divide the object into independent parts or to increase the degree of fragmentation or segmentation. Principle 13 suggests the inversion of the action(s) used to solve the problem, or to make movable parts fixed, and fixed parts movable. Concerning the principle 24, it consists to use an intermediary carrier article or intermediary process, or to merge one object temporarily with another.

The TMB is composed of one column; the application of principle 1 implies the division of the column in different zones delimited by the inlets and outlets. The goal of the future solution is to eliminate the solid circulation, in this way the application of one of the sub principles of 13 (i.e. make movable parts fixed, and fixed parts movable) imposes to fix the solid phase (make movable parts fixed). On the other hand, if the solid becomes static, inlets and outlets have to permute, in a rotating way, at



Fig. 8. Simulated moving bed.

fixed time interval (make fixed parts movable). The proposed solution consists in the simulation of liquid and solid counter flows by permutations (rotation) of inlets and outlets (toward the liquid flow direction). This improvement of the TMB arises in the Simulated Moving Bed (SMB), illustrated in Fig. 8.

With this possibility, a solution is proposed and has to be implemented and tested before to be retained in the case base.

5.2. Second possibility: similar case

Here we re-start the problem resolution just after the problem description. In our case base, there are numerous cases dedicated to chemical engineering and consequently a lot of them that are indexed with the previous contradiction. Of course, the problem description must be more detailed with additional features (Table 1).

In this more detailed example, we want to separate dimethylnaphthalene (DMN) isomers and more precisely the 2,6 DMN from the 2,7 DMN. 2,6 DMN is used as a feed stock to increase some performances of polyester (heat resistance, for example). Various separation techniques had been tested; distillation,

Table 2

Most similar case description

Prob	Soluti	ion	Comments	
Contradiction	IP:33	Technology	SMB	Methanol with 25% of water
	DP:19	Solid	ODS H-80 ¹	(viscosity problem)
Objective	Reduce solid circulation		Diam=4µm	β-cyclodextrin modified silica
Type Of Unit Operation	Separation	Apparatus	Din=1.2 cm	gel non effective
Operating Conditions	T=25°C, P=190 Atm	Dimensions	L=20 cm	Apparatus with 2 elements by
	F=1 ml/min	Rotating Time	455 s	zone (I to IV). Each one with
Mixture	2,6 DMN, 2,7 DMN,	Principles:	1, 13	the dimensions Din and L.
	Methanol, Water			

^aODS: octadecylsilyl modified silical gel.

Table 1		
Problem	descri	ption

Feature		Values
Contradiction :	Improved Parameter :	IP: 33
	Damaged Parameter :	DP: 19
Objective :		Reduce the solid circulation
Type of Unit Operation :		Separation
Operating Conditions :	Temperature	40°C
	Pressure	150 Atm
	Flow rate	30 ml/mn
Mixture :		2,6 DMN; 2,7 DMN

extraction or selective crystallization but they are not effective or not economical separation techniques. The whole new problem description is in Table 1. We can underline that the feature; type of unit operation, can be used as an index in the retrieved step in order to reduce the research time, i.e. the most relevant cases are selected in the subset of the separation techniques.

The local similarities measurement of a feature between the initial problem and a problem stored in the case base are calculated with formulas (2) or (3), depending of the type of feature. Nevertheless, concerning the chemical compounds in the mixture feature (very important in chemical engineering), which is a textual feature, the local similarity measurement can be refined as [8] had demonstrated. This approach measured the local similarity basing on the compounds chemicals structure. The compounds are divided into classes (and sub-classes) which are the compounds families (Esters, Ketons ...) and a hierarchical structure is built to describe the relations between classes.

During the step of design the operating conditions are not precisely well known in most of the cases, there are inaccuracies on them (we know an interval of possible values, value to not exceed . . .). In order to soften the problem description, the user can specify an imprecision on the values of the operating parameters and a relation (between, superior, equal and inferior). This imprecision is introduced in the local similarity measurement thanks to the fuzzy set theory.

Once the local similarities estimated, the global similarity is calculated thanks to Eq. (1), with more important values for the weights corresponding to the flow rate and mixture features.

As explained before, the case base is filled with Chemical Engineering example and of course there are similar cases which give the SMB solution. The most similar case is presented in detail in Table 2, with the stored problem description, the values of the features for the solutions and some comments concerning the solution (this solution comes from the study of [24]).

We can notice that there is a gap between the initial problem and the retrieved one, consequently the retrieved solution does not exactly correspond to the initial problem. This proposed solution needs some adjustments to be adapted to the initial problem. Here this adaptation is not made by the tool but it is one way for future research. For the moment the adaptation is as trivial as giving the retrieved solution without modification. It is the user with his knowledge and experience that does it with the retrieved solution as starting point. Even after adaptation, some imperfections can be corrected during the revised step and then retained in the case base.

6. Conclusion

This paper proposes a model and a tool (based on this model) to help and to accelerate innovative design. The presented model is based on the synergy between Case Based Reasoning and the TRIZ theory. On the one hand, CBR brings its ability to store and re-use rapidly past experiences (and knowledges) to solve new problems and its simplicity of use. On the other hand, the trans-disciplinarity of TRIZ permits the proposal of innovative solutions. Whatever the target problem face, in the worst case the tool proposed a direction to find a solution; this happens when no similar case is found in the case base. In the other case, there is a similar case, the tool gives the solution and a preliminary design of the technical solution.

To go further with the SMB technique, it can be improved too. Starting from the SMB and by the formulation of a new contradiction; we can add the reaction to this separation operation (process intensification) and finally find the Reactive Simulated Moving Bed (RSMB) (here again the tool can give some operating parameters in the proposed solution). It is important to notice that if we want to find RSMB starting from the TMB, we have to solve two successive contradictions and thus two different problems (in the model point of view) whereas it is the same unit operation and the same general problem. Consequently, the general problem has to be decomposed into two successive sub-problems. The current version of the tool cannot treat problems formalised by two simultaneous contradictions, we must consider them as two successive different cases. This is a limit of our synergy because complex problems are often solved by overcoming several contradictions. Nevertheless, the tool takes into account the possibility of successive contradictions by connecting them.

Consequently, the model (and the tool) has to be improved by eliminating some limits presented before and by adding new functionalities. The adaptation step is crucial for the success of a proposed solution and consequently to the acceleration of the design. For the moment the user does it himself but it can be helped in order to improve the whole process. A TRIZ tool, i.e. Substance-Field analysis, will be very useful because under certain conditions it gives more precise ways to solve problem.

This tool is the first version in the direction of our main goal, which is to propose a tool to help the user from the preliminary design until the detailed design. Here again, the adaptation step will be very important too (in the detailed design).

This tool is now tested in more complex examples in order to completely validate the whole possibilities. Another future work is devoted to the fitting of TRIZ ontologies and tools to the specific cases encountered in the Chemical Process Industry. Our idea in mind is to propose a TRIZ methodology, tools and ontologies used to help for a better management of innovation in the field of chemical engineering for process design, operation, manufacturing and in future research areas such as micro processes, security aspects, and clean processes.

References

- R. Srinivasan, A. Kraslawski, Application of the TRIZ creativity enhancement approach to design of inherently safer chemical processes, Chem. Eng. Proc. 45 (2006) 507–514.
- [2] J. Hipple, Solve problems inventively, Chem. Eng. Prog. 101 (4) (2005) 44–50.
- [3] R. Schank, Dynamic Memory: A Theory of Learning in Computers and People, Cambridge University Press, 1982.
- [4] A. Aamodt, E. Plaza, Case-based reasoning: foundation issues, methodological variations and system approaches, Artif. Intell. Commun. 7 (1994) 39–59.
- [5] R. Bergmann, J. Kolodner, E. Plaza, Representation in case-based reasoning, Knowledge Eng. Rev. 20 (2006) 209–213.
- [6] J. Surma, B. Braunschweig, Case-base retrieval in process engineering: supporting design by reusing flowsheets, Eng. Appl. Artif. Intell. 9 (4) (1996) 385–391.
- [7] T. Seuranen, M. Hurme, E. Pajula, Synthesis of separation processes by case-based reasoning, Comp. Chem. Eng. 29 (2005) 1473–1482.
- [8] Y. Avramenko, L. Nystrom, A. Kraslawski, Selection of internals for reactive distillation column-case based reasoning approach, Comp. Chem. Eng. 28 (2004) 37–44.
- [9] Y. Avramenko, A. Kraslawski, Decision supporting system for preselection of column internals in reactive distillation, Chem. Eng. Proc. 44 (2005) 609–616.
- [10] A. Kraslawski, T. Koiranen, L. Nyström, Case-based reasoning system for mixing equipment selection, Comp. Chem. Eng. 19S (1995) S821–S826.
- [11] I. Lopez-Arevalo, R. Banares-Alcantara, A. Aldea, A. Rodriguez-Martinez, L. Jimenez, Generation of process alternatives using abstract models and case based reasoning, Comp. Chem. Eng. 31 (2007) 902–918.
- [12] J.M.P. King, R. Banares Alcantara, Z.A. Manan, Minimising environmental impact using CBR: an azeotropic distillation case study, Environ. Model. Soft. 14 (1999) 359–366.
- [13] G. Altshuller, Creativity as An Exact Science, Gordon and Breach, New York, 1984.
- [14] K. Rantanen, E. Domb, Simplified TRIZ: new problem solving applications for engineers and manufacturing professionals, St. Lucie Press, Boca Raton, 2002.

- [15] Y. Salamatov, TRIZ: The Right Solution at the Right Time, Insytec, The Netherlands, 1999.
- [16] J. Terninko, A. Zusman, B. Zlotin, Systematic Innovation: An introduction to TRIZ, St. Lucie Press, Boca Raton, 1998.
- [17] J. Hipple, 40 Inventive Principles with Examples for Chemical Engineering, 2005 (http://www.triz-journal.com/archives/2005/06/index.htm) (Consultation: September 2007).
- [18] G. Cortes Robles, S. Negny, J.M. Le Lann, Another vision of the 40 inventive principles with applications in chemical engineering, TRIZ J. (2005) (http://www.triz-journal.com/archives/2005/12/index.htm) (Consultation: September 2007).
- [19] E. Cordova Lopez, G. Lacoste, J.M. Le Lann, Use of Altshuller's matrix for solving slag problems related to steering knuckle Part I and II, TRIZ J. (2002).

- [20] J. Hipple, Use TRIZ in reverse to analyse failures, Chem. Eng. Prog. 101 (5) (2005) 48–51.
- [21] G. Cortes Robles, Management de l'innovation technologique et des connaissances: synergie entre la théorie TRIZ et le Raisonnement à Partir de cas, Ph.D. Thesis, INPT-ENSIACET, 2006 (in French).
- [22] Y.I. Lim, S.B. Jorgensen, A fast accurate numerical method for solving simulated moving bed (SMB) chromatographic separation problem, Chem. Eng. Sci. 59 (2004) 1931–1947.
- [23] L.S. Pais, J.M. Loureiro, A.E. Rodrigues, Modeling strategies for enantiomers separation by SMB chromatography, AIChE J. 44 (3) (1998) 561–569.
- [24] Y. Dae Kim, J. Kee Lee, Y. Sang Cho, The application of simulated moving bed chromatography for separation between 2,6- and 2,7-dimethylnaphthalene, Korean J. Chem. Eng. 18 (6) (2001) 971–976.