Process synthesis using the exergy load distribution method

Enrique Mateos Espejel, Luis G. Ríos Casas*, Alejandra Alarcón García, Rocío del C. Chavela Guerra
Universidad de las Américas, Puebla. Chemical and Food Engineering Department,
Ex. Hacienda Santa Catarina Mártir. San Andrés Cholula, Pue. C.P. 72820.
Tel. (222) 229 21 26. Fax: (222) 29 27 27. E-mail: lrios@mail.udlap.mx

ABSTRACT

The objective of this work is to develop a systematic algorithm that takes into account the exergy load distribution method, proposed by Sorin et al 1992, for making the optimal synthesis of a chemical process from a superstructure. In this way, it is possible to find the optimal topology and operational condition based in the one that has the bigger exergetic contribution A_i, to the global efficiency of the process. The algorithm is applied in the hydrodealkilation of toluene process (HDA) as the base case. This algorithm will be the base of computer software, which in a future is intended to make the synthesis.

INTRODUCTION

One of the principal activities of the process engineering is the synthesis, which trough the years has been developing different methodologies for this purpose. An example are the heuristic rules, Douglas, 1988, which are based in previous experience, being really important in the way of defining the necessary superstructure for later making the synthesis (an example can be the synthesis of separation systems as shown by Douglas, 1995). The problem with the heuristic method is that rules contradict each other sometimes, because it eliminates alternatives without a quantitative evaluation, making probable that the optimal reached may not be the real optimal.

Another way of making synthesis is by the mathematical programming (linear or no linear). This kind of synthesis began to be developed at the end of the 70's. The problems of heat integration, for example, were solved making lineal an objective function (that could be minimizing the cost or maximizing the efficiency) with its restrictions, that generally were material and energy balances, by this way it was easier to get a solution, an example can be seen in Grossmann et al, 1983. But as the time has passed and the technology and research have advanced the problem can be taken in a real way, so now the restrictions and the objective function are not lineal, being the principal problem the search of the convexities, for getting the optimal solutions. A variety of techniques for solving the problems in this way are shown in Grossmann et al, 2004. This kind of solution has included many problems of the chemical engineering, like: heat integration, optimal synthesis and dynamic aspects. This method is good because if the problem is planned in a right way and it has the tool to solve the problem, it can be trusted that the solution found is the best alternative for fulfill the objective function and restrictions. However, the chemical engineer becomes a mathematician, for the complexity of the problems to solve.

A new way for making process synthesis has been developed in the last 15 years. It uses the exergy load distribution method, Sorin,M; Brodyansky, 1992. This method evaluates the exergetic distributions of a superstructure with different topologies and different operational conditions. The method relates the local exergetic efficiency of the individual part of the process with the global efficiency, calculating its contribution A_i to the global efficiency η_e. The efficiency involves the transit exergy Ex_{tr}, defined by Kostenko 1983, as the exergy that does not suffer any change during the process that introduced in the efficiency calculates the exergetic proficiency.

METHODOLOGY

The superstructure will be defined to the HDA process and the topologies of it will be simulated getting the material and energy balances. Then the input $Ex_{in,i}$. and the output $Ex_{out,i}$ local exergies will be calculated:

$$Ex_{in,i} = Ex(chemical)_{in,i} + Ex\ (mixed)_{in,i} + Ex(\ T,P)_{in,i} + Ex\ (Q_{transf})_{in,i} \quad (1)$$

$$Ex_{out,i} = Ex(chemical)_{out,i} + Ex\ (mixed)_{out,i} + Ex(\ T,P)_{out,i} + Ex\ (Q_{transf})_{out,i} \quad (2)$$

Then the transit exergies Ex_{tr} will be calculated by the algorithm proposed by Sorin et al 1994, calculating later the local exergetic efficiencies:

η_i is the local exergetic efficiency and is calculated as follows:

$$\eta_i = \frac{Ex_{out} - Ex_{tr}}{Ex_{in} - Ex_{tr}} \quad (3)$$

Then the primary loads $\lambda_{p,i}$, transformed loads $\lambda_{t,i}$ and the contribution A_i will be calculated:

$$\lambda_{P,i} = \frac{Ex_{P,i}}{Ex_C} \quad , \quad \lambda_{t,i} = \frac{Ex_{t,i}}{Ex_C} \quad (4)$$

$$A_i = \eta_i \lambda_{p,i} - (1 - \eta_i)\lambda_{t,i} \quad (5)$$

$$\eta_e = \sum_{i=1}^{n} A_i \quad (6)$$

$Ex_{P,i}$ primary exergy consumed locally, $Ex_{t,i}$ transformed exergy consumed locally Ex_C total primary exergy consumed globally and A_i is the local exergetic contribution to the global efficiency, which adding all of the parts of the process gets η_e the global exergetic efficiency. The greater A_i will be the discriminative in order to find the optimal topology.

RESULTS

12 topologies of the superstructure HDA (Figure 1) were simulated in ASPEN PLUS®. The exergetic balances for each topology were calculated; the exergetic distribution load was applied in order to take the decision of the optimal topology. The discriminative between topologies will be Ai, as said before. The different equipments and zones between topologies will be the ones that will be compared by their Ai.

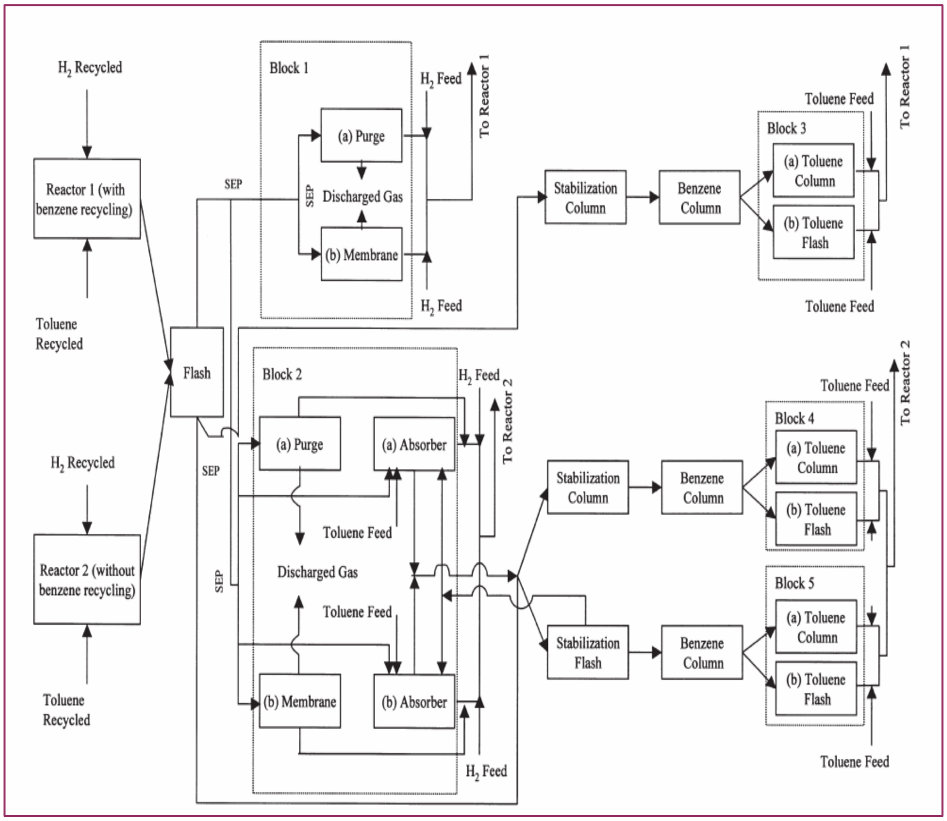


Figure 1. Topologies of the HDA process by Sorin et al, 2000.

The topologies were put face to face in order to find the optimal, beginning by group 4:

Decision 1: between the purge and the membrane, group 4:

Equipment	Efficiency	Primary load	Transformed load	Ai
1b) purge and membrane	0.0402778	0.001946909	3.47E-13	7.84E-05
1a) Purge	0.0240898	0	2.69E-05	-2.63E-05

Membrane is chosen because it has a greater Ai.

Decision 2: Between the purge with absorber and membrane with absorber, group 4.

Equipment	Efficiency	Primary load	Transformed load	Ai
2a) Purge and absorber	0.39203717	1.79E-08	1.25E-14	**7.02E-09**
2b) membrane and absorber	0.17159972	0.003750001	1.41E-05	**0.000631**

Membrane with absorber are chosen because of a greater Ai

Decision 3: For the group 4 it has to be chosen from group 5 between a column or flash of toluene.

Equipment	Efficiency	Primary load	Transformed load	Ai
3a)Tower B12	0.2567042	0.001029185	0.000585457	-0.000171
3b) Flash B12	0.154488	0.000494748	0.000444536	-0.0002994

The tower of toluene (B12) is chosen because of a less negative contribution to the global efficiency.

Decision 4: For the options of a purge with absorber and membrane with absorber that uses a stabilization column, it has to be chosen from group 5 between a column or flash of toluene.

Equipment	Efficiency	Primary load	Transformed load	Ai
4a) TowerB12	0.405697319	0.002889103	0.001969134	**1.84E-06**
4b) Flash B12	0.082046123	0.002626529	0.002003039	**-0.0016232**

The tower of toluene (B12) is chosen because of a less negative contribution to the global efficiency.

Decision 5: For the options of a purge with absorber and membrane with absorber that uses a stabilization flash, it has to be chosen from group 5 between a column or flash of toluene.

Equipment	Efficiency	Primary load	Transformed load	Ai
5a) Tower B12	0.047537932	0.00330967	0.002291525	**-0.0020253**
5b) Flash B22	0.037579469	0.003160682	0.002353113	**-0.0021459**

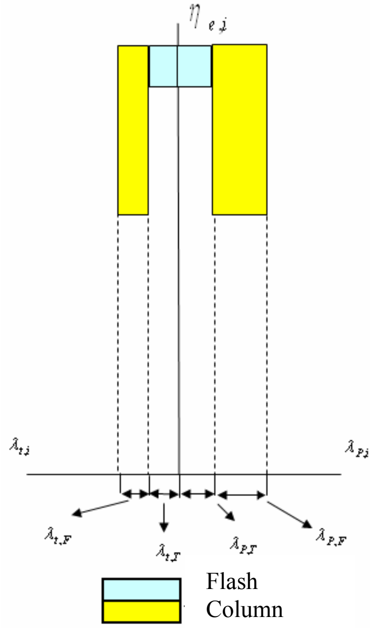
The tower of toluene (B12) is chosen because of a less negative contribution to the global efficiency.

Decision 6: For the option purge with absorber and membrane with absorber it should be chosen between the one with a stabilization flash and c. of toluene (decision 5), and the one with a column stabilization and c. of toluene (decision 4).

Equipment	Efficiency	Primary load	Transformed load	Ai
6a) Absorberr, stabilization flash	0.946556441	0.012395635	0.005129527	**0.0120073**
T. benzene,T. toluene				
6b) Absorberr, stabilization column	0.584211664	0.021704314	0.007933405	**0.0159785**
T. benzene,T. toluene				

Stabilization column is chosen because a greater Ai.

Figure 2. Diagram of exergetic contributions of decision 6.



Decision 7: It should be chosen between the membrane (decision 1) with its separation train (stabilization column, benzene tower and toluene column (decision 3)) and the membrane with absorber (decision2) with its separation train (stabilization column (decision 6), benzene tower and toluene column (decision 3)).

Equipment	**Efficiency**	**Primary load**	**Transformed load**	**Ai**
7a) purge and membrane	0.0402778	0.0019469	3.47E-13	**7.84E-05**
7b) membrane and absorber	0.1715997	0.00375	1.41E-05	**0.0006319**

The membrane with absorber is chosen because of a greater Ai. So this is the optimal topology, got by the systematic methodology and the exergy load distribution method.

The figure 3 shows the exergetic load diagram for the 7th decision, which is the optimal one for the superstructure HDA. In this figure it can be seen that the contribution Ai is the difference between two areas of two rectangles, one formed by the primary load $\lambda_{p,i}$ as the base and the $\eta_{e,i}$ as the height. And the other one y formed by the transformed load $\lambda_{t,i}$ as base and $(1 - \eta_{e,i})$ as height. For this case the area of the membrane with absorber was greater than the one with only the membrane, so this was chosen as the optimal. The Table 1 shows the contributions of all the parts of the final topology and the figure 4 shows it. The calculation can be done by equipment or by different zones of the plant as shown in the table.

For this case, at the end it was decided between all the separation trains that in the case of the final topology are the membrane, the absorber and the 3 tower. But the previous decision take into account only equipment.

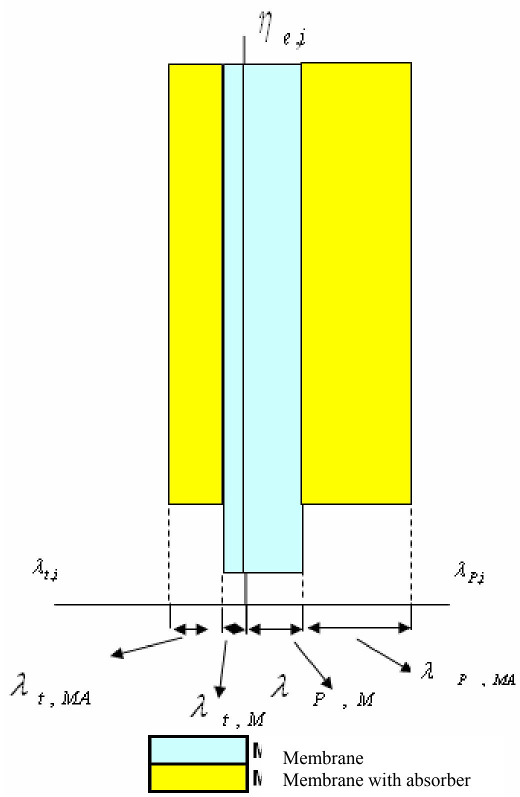
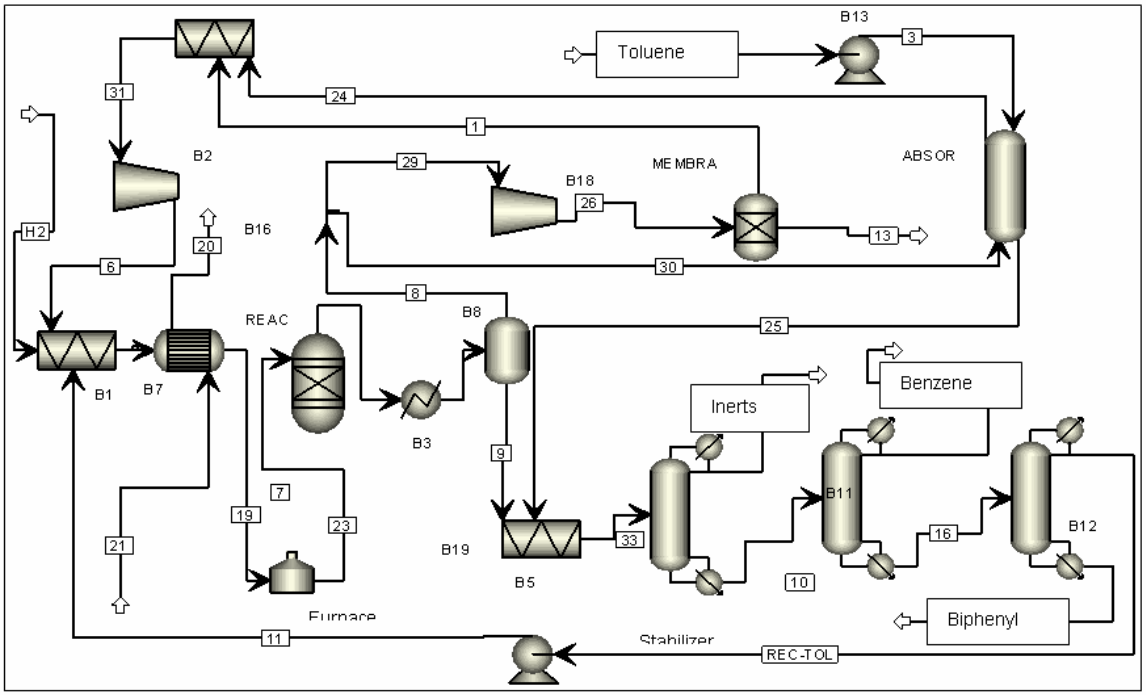


Figure 3. Diagram of exergetic contributions of the last decision

TABLE 1. Local exergetic contributions and the global efficiency of the optimal topology chosen

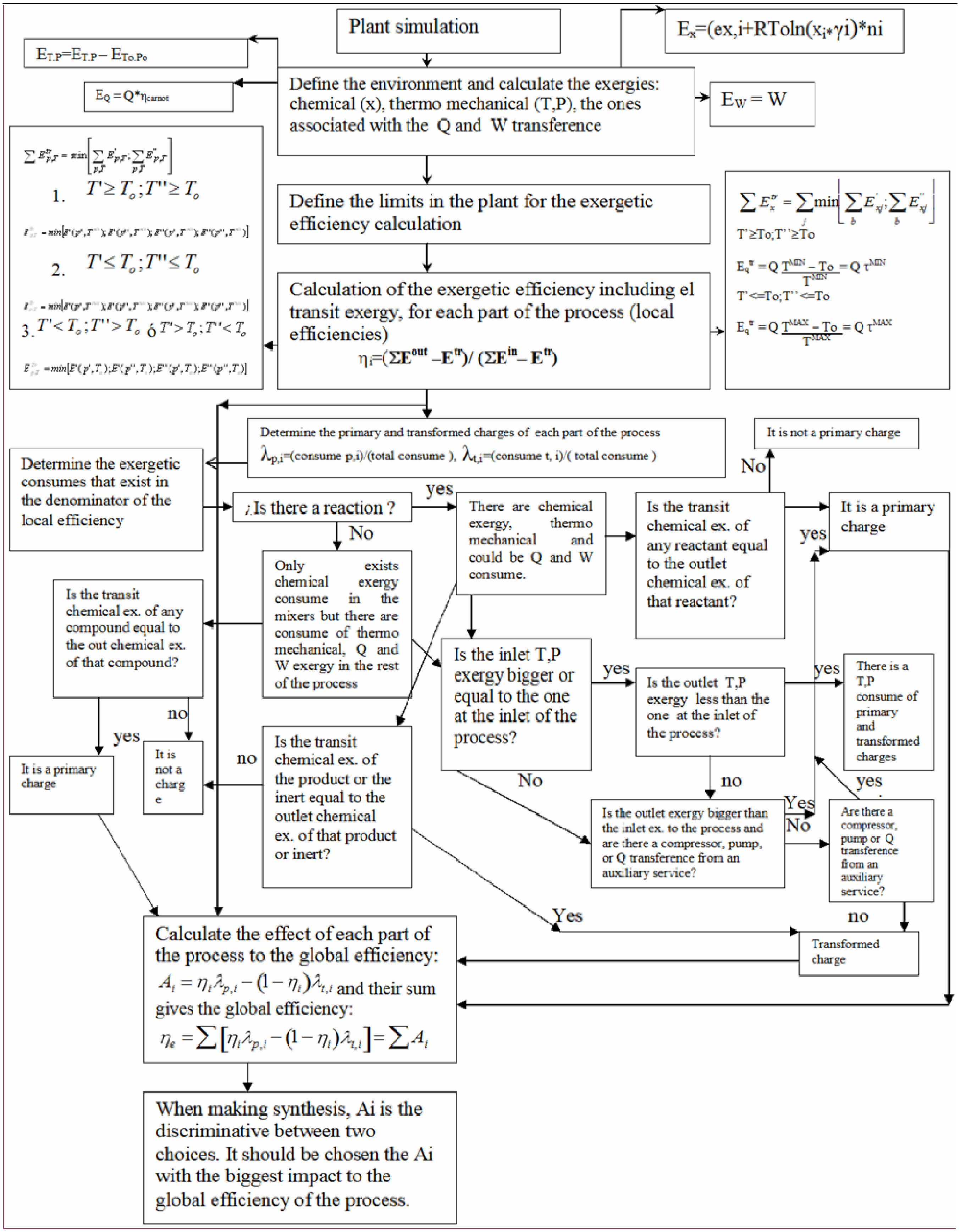
Equipment	**Efficiency**	**Primary load**	**Transformed load**	**A_i**
Mixer B1	1.00000E+00	7.21E-04	1.00E-04	7.21E-04
IC B7	6.94066E-01	1.01E-02	0	0.00E+00
Reactor	9.92918E-01	9.22E-01	7.19E-04	9.15E-01
Flash B8	9.06E-01	1.52E-06	1.9319E-03	-1.81E-04
Stabilizer	4.69E-01	1.44E-02	3.80E-04	6.56E-03
IC B3	.0124903	0	4.59E-02	-4.53E-02
Tower B11	2.55E-01	5.84E-03	7.94E-03	-4.42E-03
Tower B12	4.74E-02	3.29E-03	2.28E-03	-2.015E-03
Efficiency pump B5	0.809136039	1.70E-04	0	1.38E-04
Efficiency compressor B2	.7626	1.11E-03	0	8.44E-04
Efficiency furnace Carnot	0.849933815	3.93E-02	0	3.34E-02
Membrane and absorber	1.72E-01	3.75E-03	1.41E-05	6.32E-04
			Global efficiency	9.13E-01

Figure 4. Final topology



And all this steps for making the synthesis in this way were integrated in a final algorithm defined in the figure 5, since the beginning of the simulation to the final decision of finding the optimal topology. The only thing that has to be done first is to choose a superstructure for the one it wants to make synthesis.

Figure 5. Final algorithm.



CONCLUSIONS

The advantages of this method is that between several topologies and operational conditions it can be found an optimum, but the most important is that our principal parameter is the exergy, the potential of doing work. So the correct definition of the exergetic coefficient with the introduction of the transit exergy and the calculation of the exergetic contribution is the base for knowing the proficiency of equipment or a part of the process. This form of making synthesis is not ambiguous and does not need heuristic rules or difficult mathematics.

The proposed methodology could be incorporated to a simulator or an external modulus that allows making the synthesis of different topologies in base of the exergetic proficiency. The method of exergy load distribution is a global concept that can be applied in all cases, so the important of it. The only thing that needs is the right understanding of the process and the exergetic consumes of each part of it.

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NOTATION

General

A	Exergetic contribution
Ex	exergy
Q	heat
T,P	termomechanical

ŋ	efficiency
λ	exergy load

Subscripts

i	Pure component I, region or zone
e	global
tr	transit
transf	transferred
P	primary
t	transformed
C	Globally consumed