MODELING AND PROCESS OPTIMIZATION: AN APPROACH USING ASPEN PLUS AND MATLAB IN THE ENERGY INTEGRATION STUDY OF DISTILLATION COLUMNS

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Abstract. The present work deals with the methodology which creates the integration and the communication between different software; we focus on the Aspen Plus® simulator, MATLAB® and Excel® case. Such software interconnection represents an important objective, since it is not possible to find all the desired features in single software. As a study case, we are considering the reduction of energy consumption in the separation of a benzene-toluene mixture; a comparison between a classic distillation column and a Heat Integrated Distillation Column (HIDiC) is performed. Simulations of HIDiC and conventional columns were carried out in Aspen Plus and energy optimization of HIDiC was implemented in MATLAB. Excel is used only for communication purposes between software. As a result, the required energy in the HIDiC case is reduced by 31.25 % in respect to a conventional column with the same number of theoretical plates.

Keywords: Integration between software, distillation, HIDiC.

1. Introduction

In process modeling, it is not always possible or appropriate to perform the design and the optimization using a single software. As an example, in the case of the Aspen Plus simulator, there is the option to create templates from a friendly graphical user interface. In programming terms, a major timesaving can be obtained using vector-based software language like MATLAB. This one also provides library functions (toolbox's that are a set of functions for specialized areas such as optimization). Thus, in some cases, the simultaneously use of Aspen Plus and MATLAB results in a highly productive combination in design, modeling and process optimization (Fontalvo, 2014). However, it is required a communication interface program between the respective software.

In this study, the methodology integration between Aspen Plus and MATLAB has been programmed in Visual Basic (Excel) and applied to attain reduction of energy consumption considering the separation of a benzene-toluene mixture by distillation. The comparison was made between a classic distillation column and a column with internal integration of energy (HIDiC) considering the same total number of plates in each configuration.

Basically, the communication structure between MATLAB, Excel and Aspen 7.0 was used as shown in Fig. 1.

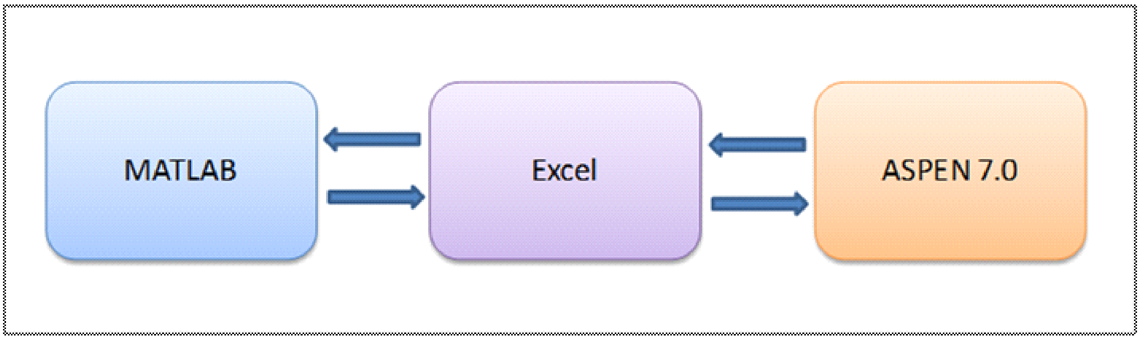

Fig. 1. Communication structure between the MATLAB, Excel and Aspen software

In this way, MATLAB does not interact directly with Aspen, but indirectly through Excel. In Fig. 1, arrows indicate a two-way communication between the software, which allows reading and writing data from any of the programs.

In the solution procedure of the HIDIC problem, MATLAB acts as the master program while Aspen and Excel operate as slaves. A large part of the calculated process variables in Aspen can be accessed by Excel using the object Variable Explorer, as shown in Fig. 2.

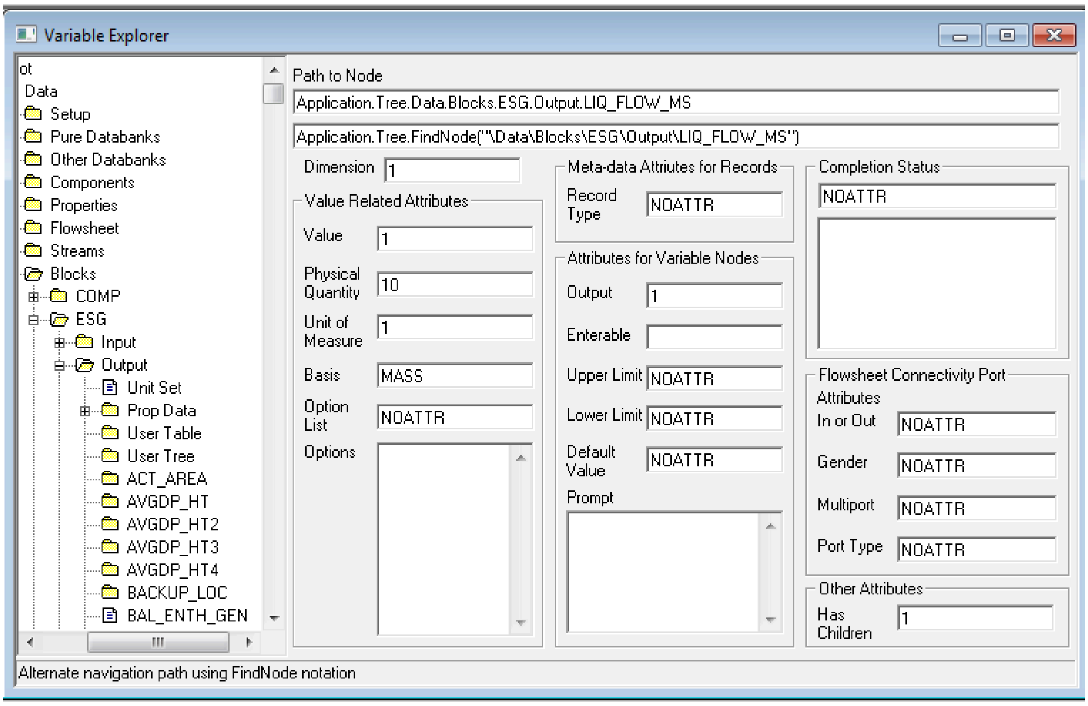

Fig. 2. Aspen Variable Explorer

In the case of Fig. 2, as an example, the path for accessing the variable mass flow rate in the stripping column is '\Data\Blocks\ESG\Output\LIQ_FLOW_MS'. In this case, the object name ESG is used to define the stripping column in the Aspen simulation file.

A simplified version of the Aspen Variable Explorer it was created in MATLAB as a list of variables containing the access path and the respective name.

2. MATLAB Communication Interface

In MATLAB you can use a series of functions to access data and to interact with Excel.

The main function is called "Run" and it is used to run functions implemented in Visual Basic (VB) on Excel, which allows data communication between MATLAB and

Aspen, as it will be described in section 4. An example for the Run function is shown below.

```
retorno = excelObject.Run('NomeFunção',param1,param2);
```

Run is a connection object function (*excelObject)* whose parameters are described in the following lines. The first parameter is represented by the function name, accessed by the VB; then the other parameters of the selected function can be send. In the example, shown earlier, we have two parameters. You can also return values (scalars) or an entire vector.

The communication between software starts with MATLAB through the creation of a server object related to Excel.

```
excelObject = actxserver('Excel.Application');
```

Then the created object has to be connected to a particular Excel file. It is worth noting that the file must contain the communication functions to access Aspen.

```
excelObject.Workbooks.Open(NomeArqExcel);
```

After that the connection object becomes visible, the Excel file is opened.

```
excelObject.Visible = 1;
```

Finally, a communication object between Aspen and Excel is created, where the NomeArqAspen parameter is the name of the modeling file in Aspen.

```
excelObject.Run('inicializacao',NomeArqAspen);
```

When the communication object is no longer required it should be deleted. This can be done by the following commands.

```
excelObject.Quit;
```

```
excelObject.delete;
```

3. Communication functions implemented in Excel

Using the Visual Basic software, contained in Excel (see Fig. 3), it is possible to write functions and subroutines as “Macros”. A file with extension ".xlsm", that allows the correct operation of the Macros, it was created. There is no need to implement any other code or insert additional information in the spreadsheets.

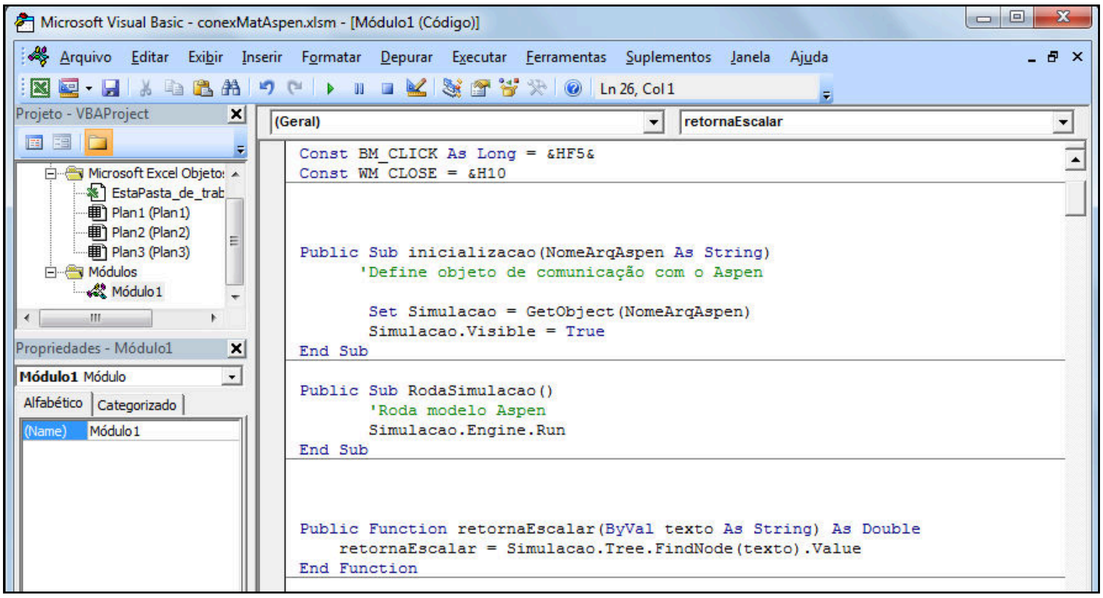

Fig. 3. Visual Basic interface contained in Excel

Two methods (functions) were implemented in Excel for data reading (from Aspen to MATLAB) and two subroutines in order to define parameters from MATLAB, as shown below:

1) `Public Function retornaEscalar(ByVal texto As String) As Double`

2) `Public Function retornaVetor(ByVal texto As String) As Variant`

3) `Public Sub DefineEscalar(ByVal texto As String, ByVal valor As Double)`

4) `Public Sub DefineVetor(ByVal texto As String, Vetor() As Double)`

The functions 1 and 2 (retornaEscalar and retornaVetor) are used for data reading and the subroutines 3 and 4 (DefineEscalar and DefineVetor) have been created for data writing. In all the functions, the "texto" parameter indicates the variable to be set or written.

It is noteworthy that the methods 1-4 are called in MATLAB from the Run function, as described in Section 2.

The first and third functions are scalar, while the second and fourth are vector-valued ones. The latest function, for instance, directly allows to access variables that are vectors in Aspen. As an example, the temperature profile in a distillation column is a vectorized variable that can be accessed directly from a single call function. The advantage of using vectorized functions consists in the execution speed, that is higher if compared to the implementation of the same functionality in scalar form.

4. Energy integration in distillation columns: minimizing power consumption using HIDiC methodology

Several technologies have been developed to improve thermodynamic efficiency of distillation process. HIDiC process stands out for combining the advantages of the other methods such as vapor recompression and diabatic operation. Furthermore, it has been proved that the HIDiC process provides better results in energy reduction compared to conventional columns, considering the same separation requirements.

The process consists of an inner arrangement of a conventional distillation column, where the rectifying and stripping sections are separated in different columns. The rectifying section operates at a higher pressure and temperatures than the stripping one. In order to increase the heat recovery, the column sections are arranged concentrically, with the rectifying one internal to the stripping one.

Due to the necessity of a pressure difference between the stripping and rectifying sections, a valve and a compressor must be included in order to allow the transference of vapor and liquid streams between the sections of the column as shown in the Fig. 1.

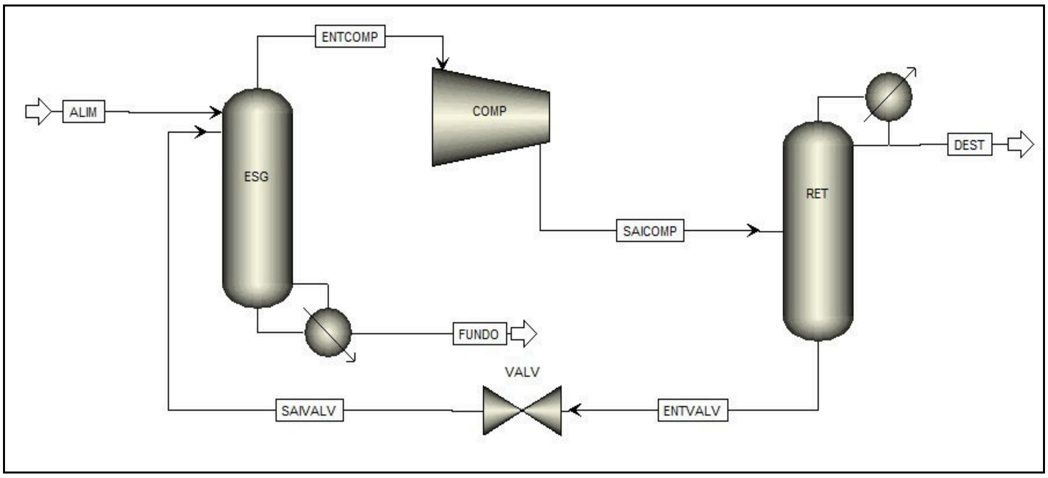

Fig. 1 – Illustration of a HIDiC column in Aspen software

The design of a HIDiC is more complex than a conventional column; anyway, the information gathered from the conventional design can be used as a set of initial parameters for the HIDiC design process. The same number of plates in the rectifying and in the stripping sections, as well the feed location are usually considered in the two types of columns. Then it must be determined the range of pressure in the compressor to ensure the thermodynamic feasibility (the plates of the rectification section should provide higher temperatures than the respective integrated plates in the stripping section). The next step consists in choosing the HIDiC type of project, such as a constant heat flow or a heat exchange area (Suphanit, 2010).

Lastly, the operation pressure as well as the respective areas of heat transfer between the plates, in order to minimize the energy consumption, must be determined. In addition, the HIDiC design should provide hydraulic viability, i.e., the calculated heat exchange area must be compatible with the dimensions of the column.

4.1. Case Study

In this work, a benzene-toluene mixture was chosen in order to compare the energy performances of a conventional and of HIDiC columns. The input data as well as the top and bottom streams specifications are shown in Table 1.

Table 1. Feed specifications, bottom and top products considered in the simulation of conventional column and HIDiC project.

<table>
<tr><td colspan="3">Feed stage</td></tr>
<tr><td>Temperature (ºC)</td><td colspan="2">75</td></tr>
<tr><td>Pressure (atm)</td><td colspan="2">1</td></tr>
<tr><td>Molar composition</td><td colspan="2">50 % benzene
50 % toluene</td></tr>
<tr><td>Molar flow (kgmol/h)</td><td colspan="2">100</td></tr>
<tr><td colspan="3">Output specifications</td></tr>
<tr><td></td><td>Top</td><td>Bottom</td></tr>
<tr><td>Molar composition</td><td>95 % benzene
5 % toluene</td><td>5 % benzene
95 % toluene</td></tr>
<tr><td>Molar flow (kgmol/h)</td><td>50</td><td>50</td></tr>
<tr><td colspan="3">Columns specifications</td></tr>
<tr><td></td><td>Conventional</td><td>HIDiC</td></tr>
<tr><td>Number of stages</td><td>26</td><td>13 stripping
13 rectification</td></tr>
<tr><td>Feed stage</td><td>13</td><td>First stage on the top of stripping section</td></tr>
</table>

In distillation columns simulations (conventional and HIDiC) using Aspen it was used the equilibrium stage model (Holland, 1981) in which it is assumed that the liquid and vapor streams that leave a particular stage are in thermodynamic equilibrium.

The Peng-Robinson equation (Peng and Robinson, 1976) was used for the phase equilibrium calculation. This model accurately describes the phase equilibrium phenomenon for hydrocarbons under high pressure.

For the performance comparison between conventional column and the HIDiC an objective function (Eq. 1) normally used in the energy integration projects evaluation (Iwakabe *et al*., 2006) is used.

The factor "3" multiplying the term Q_{Comp} has been introduced since there is a difference between the amount of electricity supplied to the compressor and the required equivalent thermal energy: the ratio is 1:3.

$$Q_{Total} = Q_{\mathrm{Re}b} + 3Q_{Comp} \tag{1}$$

where:

Q_{Total} = Total power requirement (estimated);

Q_{Reb} = Reboiler required power;

Q_{Comp} = Compressor required power.

In Eq.(1) only the energy consumption from the columns operation is considered.

More elaborated objective functions can be described in terms of cost or return on investment (Gadalla *et. al.*, 2007). In the latter case, the economic issue should be explicitly incorporated.

In the evaluation of the performance the reboiler duty of the conventional column must be compared with the reboiler duty and compressor load (Eq (1)) of the HIDiC one. Obviously, Q_{Reb} will be lower in HIDiC, however, the energy integration design maybe no economically feasible due to the demanded consumption on the compressor.

4.2 Numbering for the identification of the plates and of the equilibrium stages in the rectification and stripping columns

In Aspen, the numbering of equilibrium stages follows the top-down direction of the column according to the following convention:

- Rectification column: Stage 1 corresponds to the condenser. Stages 2-13 are the column plates;
- Stripping column: Stages 1-12 are the column plates. Stage 13 is the reboiler.

In Fig. 4 the illustration of the numbering used by Aspen is shown.

Energy integration only occurs between plates of different columns, but not between a plate and the reboiler or a plate and the condenser. Thus, there are 11 plates which are carrying out the energy integration between the two columns, which correspond to the 2-12 stages.

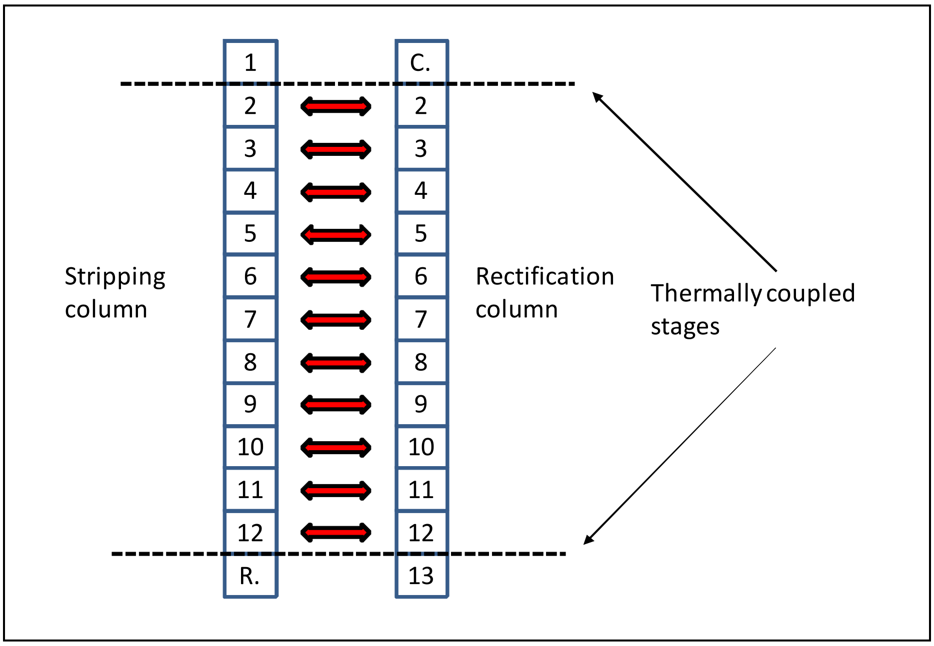

Fig. 4. Numbering of the plates and equilibrium stages in HIDiC

4.3. Determination of Thermodynamic Viability

The first part of the project deals with the validation of the system without heat transfer (without energy integration). The meaning of this step is that if there is no thermodynamic viability for the zero heat flow case this will not occur for any other condition that considers energy integration.

A thermodynamic feasibility study as a function of the pressure variation in the 1.1 to 2.5 atm range is shown in Fig. 5. For each value of the pressure (black dots), the temperature profiles in the rectification and stripping column were calculated. In order to obtain thermodynamic feasibility, we need to find the lowest value for the pressure that guarantees a positive temperature difference between the rectification and stripping columns respectively.

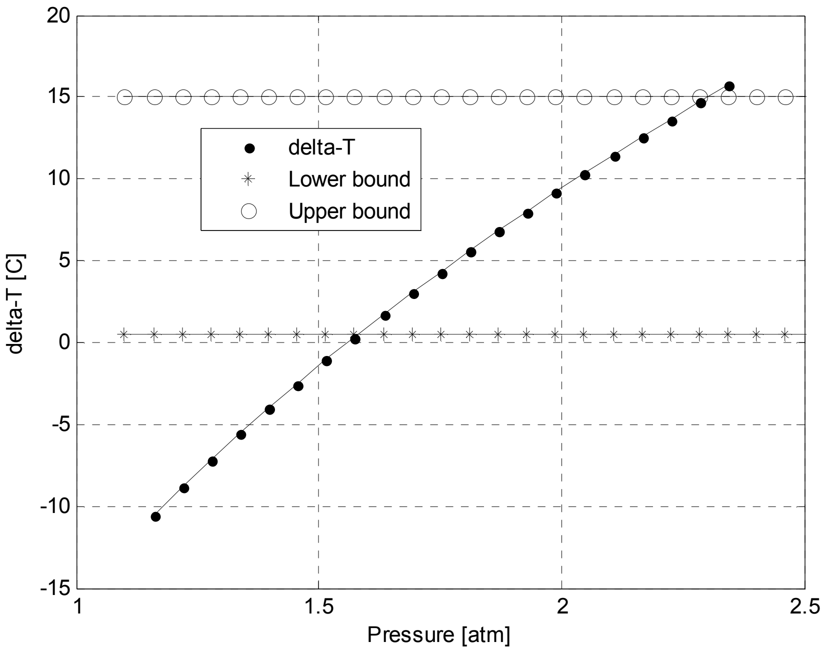

Fig. 5. Thermodynamic feasibility due to the operating pressure of the compressor.

Indeed, the lowest temperature difference between integrated stages can be negative (thermodynamic viability not achieved), this means that in some stages the temperature measured in the rectification was lower than its value in stripping column. As expected, in Fig. 5 it can be observed that this behavior occurs at low pressures. Considering a minimum acceptable temperature difference of 0.5 °C (*Lower bound*. line in Fig. 5), in order to obtain the thermodynamic viability the minimum value for the pressure is around 1.6 atm.

If the pressure increases, it is observed that the lower temperature difference between integrated stages grows directly. This behavior is expected, since the phase equilibrium in the rectification column will occur at higher temperatures due to the increased pressure.

There is no well-established standard for the maximum value pressure employed; however, the increase of the temperature difference between integrated stages in different columns leads to an increase of the heat flow between them. If the heat flows are too high, the simulator will send error messages related to the dry-plate condition or to a zero mass flow condition in one or more stages. The upper bound for the temperature difference is fixed at 15 C (*Upper bound* line in Fig. 5). At this temperature condition corresponds the higher operation pressure.

Analyzing the Fig. 5, it was determined that the feasible operating pressure range for the rectification column is 1.6 to 2.2 atm.

4.4. HIDiC Project by heat constant flux methodology

There are different ways to design a HIDiC as previously described. In this study, it was adopted the design methodology which considers constant heat flow between stages.

The constant heat flux design consists in the calculation of the pressure and of the heat flux in integrated stages in order to minimize the objective function described by Eq(1). Thus, the constant heat flux project can be considered as solution of an optimization problem subject to restrictions on the independent variables P and Q_{Stg} (heat flux per stage).

The pressure value can be located in the search range between 1.6 and 2.2 atm, in agreement with the results of the previous section.

In the heat flux per stage case, a possible search range would be between 0 and $Q_{Stg,max}$ where this is the load on column conventional reboiler divided by the number of stages energetically integrated.

In Fig. 6 it is shown the reboiler duty, the compressor duty and total estimated load versus pressure in the range 1.75 to 2.15 atm.

As expected, the load on the compressor always increases with P. The heat flow in the reboiler declines until a certain value of P as the pressure increases, then it asymptotically reach a constant value.

The minimum of the objective function (Fig. 6) represents the solution of the energy integration project and was obtained at a pressure of 1.93 atm and 71.3 kW of Q_{Stg}. The best result obtained (Fig. 7) shows temperature profiles with and without energy integration, respectively.

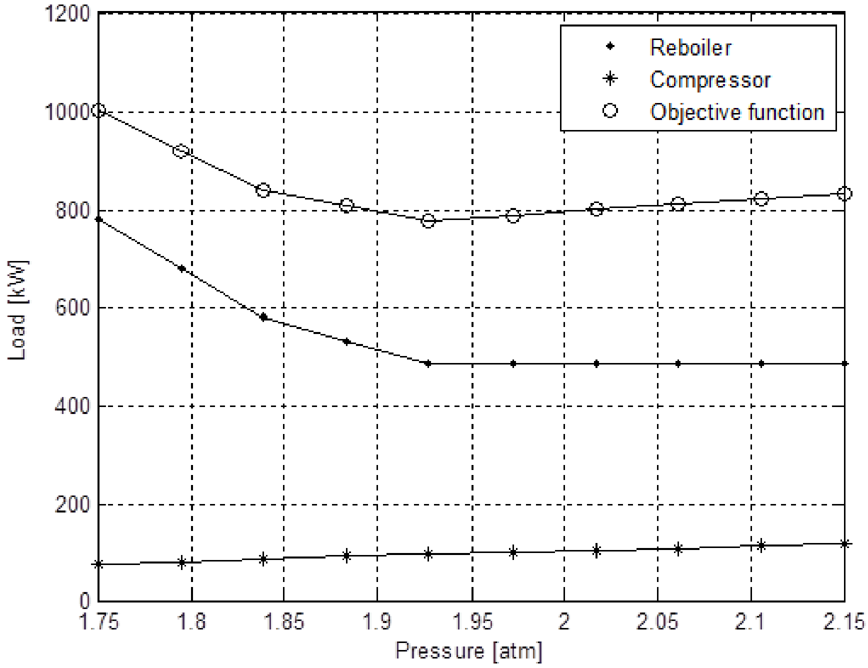

Fig. 6. Comparison between reboiler duty, compressor load and estimated total load depending on the operation pressure.

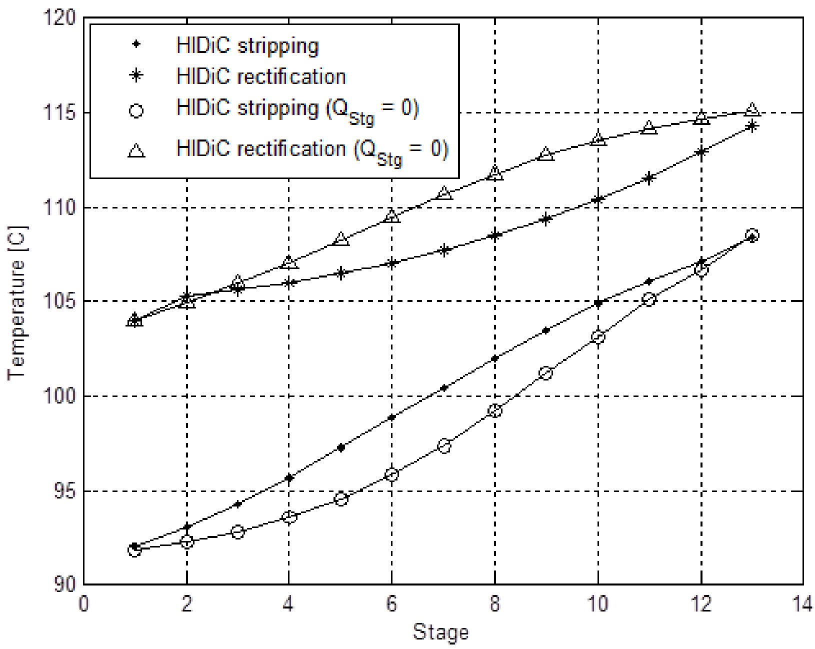

Fig. 7. Temperature profiles in the stripping and rectification columns with and without thermally coupled stages.

In Fig. 7 the temperatures related to the rectification are always higher than the stripping ones, when the respective plates, energetically integrated, are compared. Additionally it can be seen that the temperature differences between the columns are lower in the case that presents energy integration.

In general, the heat transfer between the columns will result in decreased temperature in rectification section and increased temperature in stripping column.

It is noteworthy that energy integration project should provide both hydraulic and thermodynamics viability. It is therefore considered in the HIDiC design that heat transfer area associated with each plate should be lower than the maximum calculated area.

The maximum area associated with a plate for heat transfer was calculated using the Fair correlation (Kister, 1992) and the methodology proposed by (Gadalla, 2007). In order to prevent flooding, the minimum diameter for the rectification and stripping columns is obtained by the first correlation. Knowing the diameter of the columns, the methodology estimates the maximum area compatible with the columns dimensions.

A summary of the results obtained with the HIDiC project at constant heat flux is provided in Table 2.

Table 2. Summary results of the energy integration project

Optimized variables	
Pressure (atm)	1.95
Heat duty per stage (kW)	71.89
Results	
Compressor load (kW)	97.56
Reboiler duty (kW)	485.89
Objective function (kW)	778.58
Total heat transfer area (m^2)	107.72

The energy consumption in the conventional column was 1132.48 kW. For the same number of plates in a HIDiC column the consumption was 778.58 kW, considering the contributions of the reboiler and compressor. This implies an energy reduction of 31.25 %.

5. Conclusion

The methodology of integration between MATLAB and Aspen Plus has been successfully implemented in Visual Basic (Excel), being applied in reduction of energy consumption considering the separation of a benzene-toluene mixture.

In comparison with the conventional column, an energy consumption reduction of 31.25 % was obtained using a HIDiC with the same number of plates for a benzene-toluene mixture.

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