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# Preliminary Conceptual Design of a Distillation Column with Energy Integration (HIDiC)

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Several procedures have been defined for the success in the design of conventional distillation columns. Into these procedures, definition of operation pressure, reflux ratio, minimum number of stages, feed stage are key steps. For non-conventional columns, such as Heat Integrated Distillation Columns (HIDiC), the complexity of the system adds difficulties to the definition of starting values for design and operational variables. The objective of this study is to propose a methodology for the preliminary conceptual design of Heat Integrated Distillation Columns considering exergetic efficiency. The methodology considers five global steps to achieve a rational design for a concentric HIDiC. It starts with the simulation of the separation in a conventional distillation column; then, with the obtained results, the HIDiC simulation is carried out, either for top or base configuration which depends on the estimation of the number of stages for each section. Into the HIDiC simulation, pressures definition must consider a minimum temperature difference criterion. Once achieved, the respective HIDiC configurations are simulated and the exergetic balance is performed, the results are compared for the selection of the configuration. The design procedure and simulations are applied for the separation of a propylene-propane binary mixture. The results of the preliminary conceptual design are presented and the reduction in exergy lost for the selected HIDiC is verified by comparison against a conventional distillation column.

## 1. Introduction

Distillation is one of the most energy intensive unit operations in the chemical industries (Gorak & Sorensen, 2014). The low thermodynamic efficiency of distillation operations can be explained by the high temperature differences between the condenser and the reboiler, which generate a very low second-law efficiency and hight exergy loss. Many distillation configurations have been proposed to increase its thermodynamic efficiency, such as dividing wall column (DWC), vapor recompression column (VRC), diabatic distillation, and internally integrated distillation column (HIDiC). All these configurations have been compared by Kiss et al., (2012) and recommended applicability ranges for each distillation technology.

Mah et al., (1977) introduced the HIDiC concept to improve the energy efficiency in distillation. HIDiC are especially suitable for distillation of close boiling point mixtures (Kiss & Olujić, 2014). However, there are issues to solve before HIDiC can be applied to industrial scale such as hydraulic behaviour (Gadalla, et al., 2007), the heat and mass transfer characteristics associated with the internal heat integration and the geometry of these type of columns (de Rijke, 2007), as well as more information to select suitable HIDiC configurations for different types of systems (Mancera et al., 2018).

Currently, methodologies for conceptual design of HIDiC are based on pinch and hydraulic analysis (M. Gadalla et al., 2005; M. A. Gadalla, 2009), in economic criteria to find optimal HIDiC configuration (Olujić et al., 2006; Suphanit, 2010), in heat integration maximization (Marin et al., 2018). In this work an exergy-based (exergy minimization) methodology is proposed to define the basic characteristics of HIDiC columns, as initial step for a design with least exergy losses.

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## 2. Methodology

In this section a methodology for basic HIDiC conceptual design is presented, it comprises five steps (Figure 1) to ensure the conceptual design for an exergy based HIDiC.

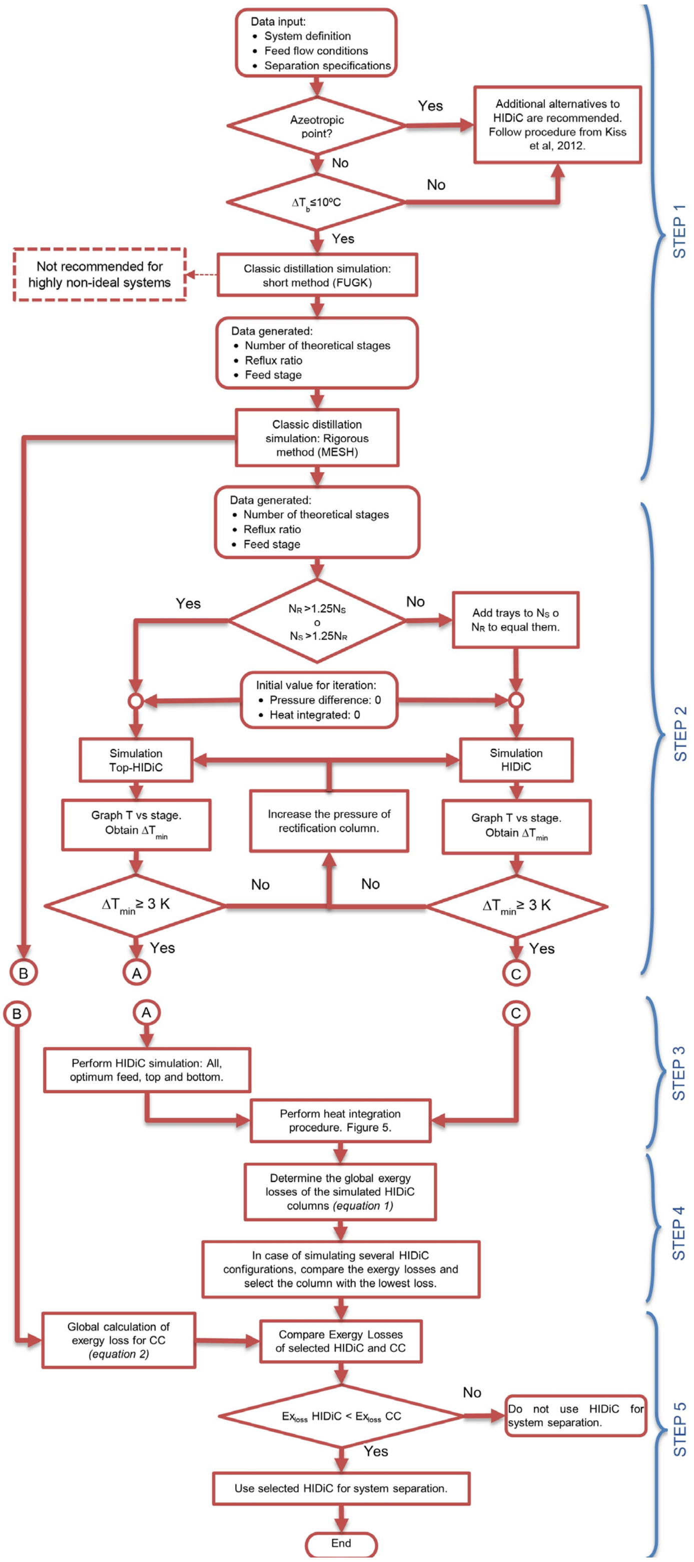


*Figure 1: HIDiC Preliminary Design Procedure Flow Chart.*

*Step 1. Characterization of the system and separation:* Binary system to purify is defined, the feed conditions ($q$, temperature, flow, composition, and pressure), and the composition of distillate and bottom products ($X_D$, $X_B$). If the mixture has an azeotropic point or if the boiling point difference $\Delta T_b$ of each component if greater than 10°C it is recommended no to use HIDiC technology and the procedure recommended by Kiss et al., (2012) should be followed; otherwise the procedure follows with a shortcut method (Fenske-Underwood-Gilliland-Kirkbride, FUGK) to estimate the number of theoretical stages, the flow ratio, the feeding stage, and the energy consumption in the condenser and reboiler. Once completed the previous stage, a rigorous method (MESH: mass-equilibrium-sum fractions-enthalpy balance equations) is used by Aspen®, without pressure drop between plates and with the pressure that reduces condensation costs, thereby obtaining initial values for HIDiC analysis.

*Step 2. Definition of HIDiC type and compression ratio:* HIDiC is simulated based on the results of Step 1. The different configurations considered are the same ones studied by Mancera et. al., (2018). If the number of stages in the rectification section ($N_R$) is 1.25 times greater than the number stages of the stripping section ($N_S$), or vice versa, a top HIDiC is simulated, otherwise a basic HIDiC is simulated, adding stages to the section with less trays to equal the number of stages in each column section ($N_R = N_S$). To define the compression ratio between the column sections, the point with the greatest temperature difference is identified for the two sections operating at the same pressure (Figure 2a) and without energy integration, with the liquid compositions at the identified point, then the pressure in the rectification zone is increased by starting with a suggested $\Delta P$ (it can come from the literature for a similar system or for the same system but in similar columns that are not HIDiC and that work with a pressure difference between the sections, e.g. VRC), in case of not having some basic information, it starts with an increase of 10%. Then a temperature vs stage plot is made to identify the minimum temperature difference ($\Delta T_{min}$) between the columns, as shown in Figure 2b. The recommended least allowed temperature difference is 3 K (Gadalla et al., 2007; Gadalla, 2009; Marin et al., 2018; Suphanit, 2010). If $\Delta T_{min}$ is less than 3 K, the pressure difference between column most be increased again. This step is repeated until $\Delta T_{min} \geq 3$ K.

*Step 3. Definition of heat distribution:* This step depends on the HIDiC type simulated in the previous step. In the case of top HIDiC, three configurations are assessed (total, optimal feed and bottom) using the pressure difference obtained in step 2 and proceeding to find the heat distribution for each configuration according to Figure 3. If the selected HIDiC type is the basic one, the heat integration is obtained using $\Delta P$ of step 2.

*Step 4. Determination of exergy loss* ($Ex_{loss}$)*:* An exergy analysis on the selected configuration is performed. In the case of simulating different configurations, the selected column will be the one with lower exergy loss.

*Step 5. Analysis of results:* Finally, in this step the exergy losses of the selected HIDiC is compared with the exergy loss of the conventional column (CC). The one with less exergy loss is selected.

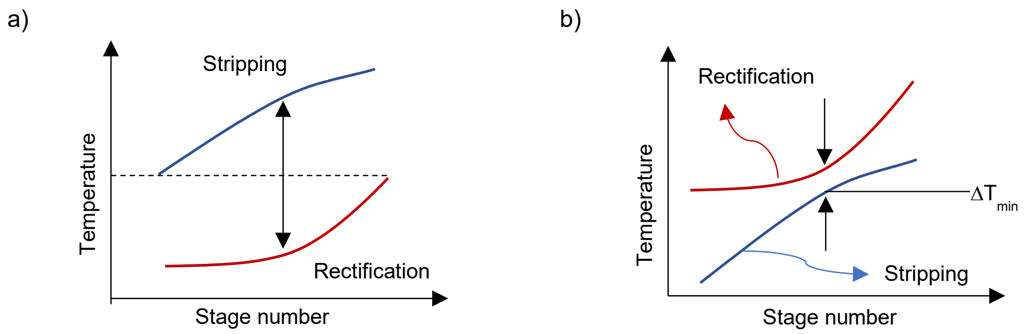


*Figure 2: Temperature profile per stage before (a) and after (b) pressure setting.*

## 3. Results

The results are presented using the propane-propylene mixture as case study.

*Step 1.*
Peng-Robinson equation of state is used to describe the phase equilibrium. A summary of the specifications is in Table 1. The $\Delta T_b$ for the system is 7.7 °C and the results from shortcut FUGK method are shown in Table 2.

*Table 1: Feed Flow specifications and separation conditions.*

| Feature | Value |
|---|---|
| Feed flow (kg/h) | 112000 |
| Fraction mol feed (propylene) | 0.50 |
| Thermal condition feed (q) | 0.37 |
| Fraction mol distillate (propylene) | 0.996 |
| Fraction mol bottoms (propylene) | 0.011 |
| Operation pressure (bar) | 11.2 |

*Table 2: Results of the short method for the case study.*

| Feature | Value |
|---|---|
| Reflux ratio | 13.83 |
| Stages rectification section | 98 |
| Stages stripping section | 54 |
| Feeding stage | 99 |
| Duty boiler (GJ/h) | 299.96 |
| Duty condenser (GJ/h) | 313.69 |
| Pressure (bar) | 11.2 |

The parameters for the conventional column simulation using the rigorous method (MESH) are based on the results obtained using the shortcut (Table 2). The outcome of the rigorous simulation, Table 3, are used as starting values to initialize the HIDiC simulation. The specifications for simulation were propylene composition in the distillate and bottom streams, varying the distillate flow and the reflux ratio.

*Step 2.*

According to the results obtained in Step 1, the number of stages of the rectification zone is greater than 1.25 times the number of stages of the stripping zone (98 vs 54). Therefore, the Top HIDiC is the best option to be simulated. The initialization parameters for the Top HIDiC are summarized in Table 4.

*Table 3: Results of rigorous method for the case study.*

| Features | Value |
|---|---|
| Reflux ratio | 17.15 |
| Stages rectification section | 98 |
| Stages stripping section | 54 |
| Feeding stage | 99 |
| Duty boiler (GJ/h) | 341.78 |
| Duty condenser (GJ/h) | 355.48 |
| Pressure (bar) | 11.2 |

*Table 4: HIDiC simulation initialization conditions*

| Features | Value |
|---|---|
| Reflux ratio | 17.15 |
| Stages rectification section | 98 |
| Stages stripping section | 54 |
| Feeding stage | 99 |
| Pressure (bar) | 11.2 |

*Table 5: Evolution of the temperature difference between column sections according to pressure difference.*

| Stripping column pressure (bar) | Rectification column pressure (bar) | Pressure difference (bar) | $\Delta T_{min}$ (ºC) | $\Delta T_{max}$ (ºC) | $\Delta T_{aver}$ (ºC) |
|---|---|---|---|---|---|
| 11.2 | 11.2 | 0 | -7.13 | -2.35 | -4.69 |
| 11.2 | 12.32 | 1.11 | -3.30 | 1.51 | -0.84 |
| 11.2 | 13.44 | 2.24 | 0.28 | 5.13 | 2.77 |
| 11.2 | 14.6 | 3.4 | 3.76 | 8.66 | 6.28 |
| 11.2 | 15.68 | 4.48 | 6.82 | 11.76 | 9.37 |

The aim of this step is to determine the pressure difference between columns to ensure a minimum temperature difference of 3 K that guarantees appropriate column operation. The simulation was run using different pressures, according to the proposed methodology, then the temperature difference in both sections was calculated. Table 5 shows the pressures assessed together with maximum, minimum and average temperature differences. The selected pressure difference (ΔP) was 3.4 bar, which generates a minimum temperature difference of 3.76 K, fulfilling the requisite. The smaller pressure difference that fulfills the conditions is selected considering the whole column cost. The reflux ratio calculated for the chosen column is 20.48 to match the separation specifications.

*Step 3.*
The simulation of different HIDiC configurations (total, optimal-feed, top, and bottom), using ΔP found in step 2, is carried out to find a proper heat integration, as shown in Figure 3. A summary of results is given in Table 6.

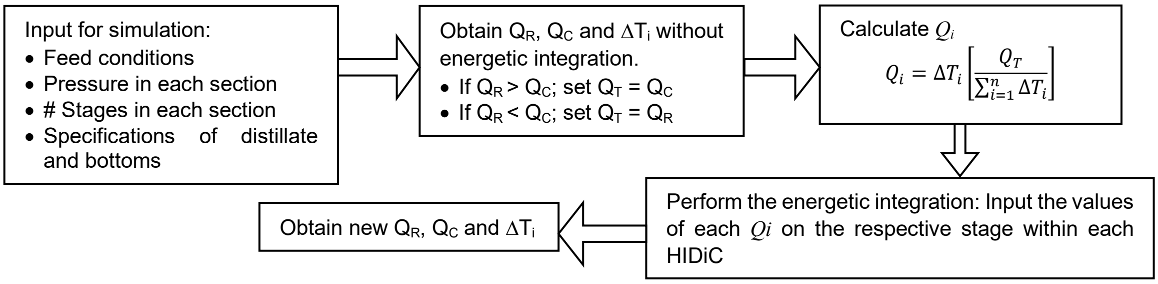


*Figure 3: Estimation procedure for heat flow distribution between rectification and stripping sections.*

*Table 6: Operational conditions of the different HIDiC configurations.*

| Features | Top-HIDiC | Bottom-HIDiC | Feed opt.-HIDiC | All-HIDiC |
|---|---|---|---|---|
| Rectification section Pressure (bar) | 14.6 | 14.6 | 14.6 – 11.2 | 14.6 |
| Stripping section pressure (bar) | 11.2 | 11.2 | 11.2 | 11.2 |
| Stages rectification section | 98 | 98 | 98 | 98 |
| Stages stripping section | 54 | 54 | 54 | 54 |
| Feeding stage | 99 | 99 | 99 | 99 |
| Trays in the Concentric Column | 97 | 97 | 75 | 97 |
| Trays in the Annular column | 53 | 53 | 75 | 53 |

*Step 4.*
The overall exergy loss of each configuration is calculated using Equation 1.

$$Ex^{loss} = S(Ex_{steam,in} - Ex_{steam,out}) + A(Ex_{cw,in} - Ex_{cw,out}) + W_{comp} + FEx_F - DEx_D - BEx_B \quad (1)$$

The results of the exergy loss in the top, bottom, total and optimal feed are shown in Table 7. It can be noticed that the HIDiC of least exergy lost is the top HIDiC, thus, this is the chosen configuration.

*Step 5.*
The exergy loss of the conventional column is obtained using Equation 2.

$$Ex^{loss} = S(Ex_{steam,in} - Ex_{steam,out}) + A(Ex_{cw,in} - Ex_{cw,out}) + FEx_F - DEx_D - BEx_B \quad (2)$$

A comparison of exergy losses of the Top HIDiC and conventional columns, Table 8, shows that Top HIDiC is more efficient (about 50 % less exergy loss) than the conventional column.

*Table 7: Exergy losses of the different HIDiC configurations.*

| Type of HIDiC | Loss exergy (GJ/h) |
|---|---|
| Top | 49.58 |
| All | 49.77 |
| Optimum Feed | 68.69 |
| Bottom | 95.64 |

*Table 8: Loss exergy from the Top-HIDiC and the conventional column.*

| Type of column | Exergy loss (GJ/h) |
|---|---|
| Top-HIDiC | 49.58 |
| Conventional | 99.32 |

## 4. Conclusions

A conceptual design methodology for analysis of columns with internal energy integration (HIDiC) was presented, the methodology considers some tools developed for conventional columns, useful heuristics for HIDiCs and conclusion obtained from results of previous works. Considering the current environmental and operational tendencies, exergy is a key criterium to assess the convenience of using non-conventional configurations for separation tasks, since this guarantees energy efficient designs. The proposed methodology contributes to develop conceptual design methodologies for thermodynamically efficient columns, a gap for the implementation of these technologies. To improve the decision procedures, it is recommended to develop design methodologies that combine thermodynamic and economic assessment of different types of HIDiC columns. For the study case, propane-propylene system, it was shown that HIDiC configurations generate more efficient separations, but an economic analysis is recommended since exergy losses in Top and Total HIDiC are similar.

## Nomenclature

| | | | | | |
|---|---|---|---|---|---|
| $A$ | Water flow (kg/h) | *Subscripts* | | min | Minimum |
| $B$ | Bottom flow (kg/h) | $B$ | Bottom stream | $n$ | Integrated tray pair |
| $D$ | Distillation flow (kg/h) | B | Boiling point | $out$ | Outlet |
| $Ex$ | Exergy (GJ/kg) | $c$ | Condenser | prom | Average |
| $F$ | Feed flow (kg/h) | $Comp$ | Compressor | $R$ | Reboiler |
| N | Stages | $D$ | Distillation stream | Re | Rectification column |
| $Q$ | Heat flow (GJ/h) | $F$ | Feed stream | $S$ | Stripping column |
| $S$ | Vapor flow (kg/h) | $in$ | Inlet | $steam$ | Steam |
| $T$ | Temperature (ºC) | $loss$ | Exergy loss | $T$ | Total |
| $W$ | Work (GJ/h) | max | Maxime | $cw$ | Cooling water |

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