ARTICLE

Efficient Exergy Analysis of Chemical Processes through Process Engineering Software

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ABSTRACT

In this work, authors present a simple methodology for computing physical, chemical and total exergies, and the exergy destruction and the exergetic efficiency of simple and complex processes by using the object linking and embedded (OLE) automation by connecting Aspen HYSYS to MS Excel VBA. For this purpose, a simple flowsheet was added to the main one with the same number of streams as that of the components. By introducing all these streams in a mixer and then consecutively conducted to a heater to condition the outlet stream, a separator and a mixer, the VBA application was able to compute the chemical exergy of the different streams of the main flowsheet. To demonstrate the procedure here described seven cases were considered: single streams, a CO_2 mixer, a cooler, a distillation column, a reactor, a multiple recirculation process, and different configurations of separating components by distillation, which can be extended to very complex processes. The former was selected to validate the methodology here proposed whereas the rest of cases were used to demonstrate the potential of the tool here developed, which in turn could be used for discriminating among different process alternatives.

Keywords: Automation; Simulators; MS Excel-VBA; Exergy analysis

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1. Introduction

Exergy analysis (ExA) has been gaining relevance in the field of energy efficiency as a powerful tool to assess degradation of energy quality or, to put in other way, to evaluate the efficiency in the use of energy [1], and has an important role to play in addressing climate change and expanding use of sustainable energy [2] since by identifying improvements and reductions in wastes and environmental impacts it can help to better understand the potential benefits of relevant measures. Paraphrasing prof. Novak: 'we are paying for the quantity of energy but we are using only the quality (Exergy) of energy' [3].

The use of ExA allows to develop new chemical processes, incorporating energy efficiency constraints to the process design stages [4]. In addition, social, environmental and economic factors play a role in the critical evaluation of a process and exergy could be considered as the property that joins everything together [5].

ExA quantifies the percentage of destroyed exergy via process irreversibilities as well as the percentage of lost exergy via process deficiencies when handling waste (material and energy) streams and might also be used as design criteria for optimization of process in order to minimize energy requirements, energy degradation and waste (material and energy) streams [1]. Among all the industrial sectors, the chemical industry is energy intensive with 33% share in total industrial energy use. Increasing cost of raw materials, infrastructure and energy increases burden on the profit margin of the chemical sector [6].

A number of studies have demonstrated that exergy analysis is a key tool in the design, analysis, and performance optimization of power plants [7–17], solar power plants [18], solar thermal power plant hybrid with designed Phase Change Materials storage [19], biomass-fired power plants [20], marine steam power plants [21], post-combustion CO_2 capture using MEA-solvent chemical absorption [22], co-firing combined power plants [23], combined cycle power plants with chemical looping technology [24] or sugarcane bagasse power cogeneration systems [25]. A comparative exergoeconomic assessment of coal-fired power plants-Binary Rankine cycle versus conventional steam cycle was recently reported [26]. On the other hand, other studies have explores avoidable carbon emissions by reducing exergy destruction based on advanced exergy analysis [27].

Many of the studies use SPecific Exergy COsting developed by Lazzaretto and Tsatsaronis [28]. It consists of a systematic and general methodology for defining and calculating exergetic efficiencies and exergy related costs in thermal systems. A detailed exergy analysis was performed for the steam reforming process of glycerol by means of a series of experiments in a bench scale apparatus [29]. A methodology for application of exergy analysis has been developed to evaluate the efficiency of pyrolysis systems for waste polymers in order to obtain different types of fuels determining optimal conditions for the processes and comparative analysis of the results [30]. Some authors have shown that the exergy efficiency of hydrogen production from steam gasification of biomass is mainly determined by the H_2 yield and the chemical exergy of biomass [31]. An exergy flows analysis in chemical reactors was also performed [32]. Exergy-based evaluation of methanol production from natural gas with CO_2 utilization [33]. Energy and exergy balances were evaluated for the units that constitute the aromatics plant of a refinery [34]. Advanced exergy analysis applied to the process of re-gasification of LNG (liquefied natural gas) integrated into an air separation process [35].

Some studies have used some simulator for computing the basic physical properties to perform the exergy analysis. Thus, an exergy study of an amine scrubber unit of a Sulphur recovery plant using methyl diethanolamine was developed in which the physical exergy was calculated through Aspen HYSYS whereas chemical exergy was calculated through a series of equations embedded in excel [36]. Recently, a visual basic application (VBA) for Microsoft Excel 2007 has been developed as a helpful tool to perform mass, energy, exergy and thermoeconomic calculations during the systematic analysis of energy processes simulated with Aspen Plus. The application read an Excel workbook containing three sheets with

the matter, work and heat streams results of an Aspen Plus® simulation. The required information from the Aspen Plus simulation and the algorithm/calculations of the application were described and applied to an Air Separation Unit. ProSimPlus was also proposed to be used in the definition of a methodology for performing exergy balances [37] and exergy efficiency evaluations [38]. A mercaptan oxidation unit of an oil and gas refinery was simulated using Aspen HYSYS V10.1 to obtain extended mass and energy balances and assessed using exergy and parametric sensitivity analysis to identify opportunities for improvement from a technical and energy point of view [39]. The exergy analysis was applied to two case studies: the base case and the resulting case from technical improvements. The global exergy efficiency, irreversibilities, exergy of utilities, and efficiencies per stage were calculated to map process equipment with the highest losses of exergy. The physical exergies were calculated during the simulation, and the chemical exergies of the different compounds that are involved in the process were gathered from the literature. The synthesis of monochloromethane production through methanol hydrochlorination plant was simulated by using Aspen HYSYS, which provided physical properties that together the chemical exergy value of process substances allowed to compute the specific physical and chemical exergies of the streams involved in the process [40]. This analysis was extended by the same authors to the methane chlorination process for methyl chloride production [41].

On the other hand, a straightforward method for calculating physical and chemical exergies of material stream was proposed and implemented in Aspen HYSYS by utilizing fifteen main user variables for material streams [42]. Such computer-aided exergy calculations would make exergy analysis more accessible in Aspen HYSYS process simulator resulting in more insight into the nature of irreversibilities associated with specific process [42]. However, the implementation of these methodologies is not easy for standard users.

The authors of this work have experience in connecting Aspen Plus and Aspen HYSYS via auto-mation. Automation is the process of linking commercial software to third parties applications built in MS Excel-Visual Basic for Applications (MS Excel-VBA), Python, Matlab, etc. and constituted a powerful tool for simulating unprecedented complex. Santos and Van Gerven [43] studied the connection methodologies of the process simulator Aspen HYSYS with four tools typically used by chemical engineers: Microsoft Excel (VBA), Matlab, Python and Unity (C#), and compared their performance results obtained in terms of accuracy of communication, time of exchange, and deviation in the results. According to our experience the best performance is similarly achieved with MS Excel-VBA and Python.

Aspen HYSYS was used together to MS Excel-VBA for simulating typical examples used in Master courses as a refrigeration process and the production of biphenyl [44] and more complex problems as the computation of azeotropes, determination of the temperature and concentration profiles inside a catalyst particle by considering the reaction and simultaneous non-isothermal internal and external diffusion phenomena, and the simulation of the thermal cracking of ethane with coke formation, among others [45]. The capability of the Automation concept by using Aspen Plus was also demonstrated for making the sensitivity analysis of the biphenyl production and the optimization without constraints of the composition of a stream from the production of cumene (design specification), and the optimization with constraints of the isomerization of nC4- to iC4- [46].

Very recently, Digital Twins based on Neural Networks for the steady state production of styrene were generated by using Aspen HYSYS and/or Aspen Plus, which were connected through a recycle-like stream via automation for solving the entire simulation flowsheet [47]. Aspen HYSYS was used for solving the pre-heating, reaction, and stabilization sections of the process whereas Aspen Plus ensured the computing of the separation and purification columns. Both alternatives led to an excellent prediction showing the capability of creating Digital Twins from and for process simulation.

In this work, authors present a simple methodology for computing physical, chemical and total exergies of simple processes by using the automation concept which is simpler than that based on the definition of user variables. This way, it was possible to compute the total exergy of material and energy streams, from the physical and the chemical ones, and then the exergy destruction and the exergetic efficiencies. Seven examples were considered to demonstrate the capability of the procedure proposed: single streams, CO_2 mixer, cooler, distillation column, reactor, different configurations of separating components by distillation, and a multiple recirculation process, which can be extended to very complex processes. The basis of this methodology has been used by the authors for designing tools for computing exergy, exergoeconomic and exergoenvironmental analysis of chemical processes through Aspen HYSYS and Aspen Plus simulations.

2. Exergy analysis

Exergy flow (in kW) is defined as the maximum power (mechanical work) obtainable when a stream reaches equilibrium with a reference external environment [1]. In the absence of nuclear effects, magnetism, electricity and surface tension, molar exergy of a stream of matter (B) can be formulated as follows [42]:

$$B = B_{physical} + B_{chemical} + B_{kinetic} + B_{potential}$$

(1)

Kinetic and potential exergies are normally negligible compared to the other two components: physical and chemical ones. Molar physical exergy of a stream ($B_{physical}$)is the work obtainable by taking 1 mol of stream through reversible process from its initial state to the state determined by the temperature T_0 and P_0 of the environment, known as reference conditions:

$$B_{physical} = (h - h_0) - T_0(s - s_0)$$

(2)

where h and s and h_0 and s_0 are the molar enthalpy and the molar entropy at its initial state and at the conditions of the environment, respectively [48]. The chemical exergy of a system is defined as the max-

imum amount of useful work that can be obtained when the system under consideration is brought from its restricted dead state to the complete dead state (both are the same) where the system is in complete thermodynamic equilibrium with the environment [48]. Changes in chemical exergy are associated to the presence of chemical reactions (e.g., combustion), mixing of constituents, and phase change. Proper exergy analysis of many industrial processes should account for these changes. Examples are electrical generation stations using combustion, fuel cells where the chemical energy of a fuel is converted to electricity through a chemical reaction, biomass gasification devices, distillation columns and petrochemical processing plants [49].

The chemical exergy for a multiphasic stream can be computed [42,48,50,51] as follows:

$$B_{chemical} = \sum_{j=1}^{Phases} \left\{ F_j \left[\sum_{i=1}^{nc} \left(z_{i_j} \left\{ (b_i^0)_j + RT_0 ln \left[a_{i_j} \left(T_0, P_0, z_{1_j}, z_{2_j}, ..., z_{nc_j} \right) \right] \right\} \right) \right] \right\}$$

(3)

where *Phases* is the number of phases in the mixture, *nc* is the number of species, F_j is molar flow of phase j in the stream, z_{i_j} is the molar fraction of i in phase j, R is the constant of gases, a_{i_j} is the activity of specie i in phase j, and $(b_i^0)_j$ is the molar chemical exergy of specie i in the phase j at obtained at T_0 and P_0. The values of the later are tabulated [51]. **Table S1** collects the value of the molar chemical exergy of all the species considered in this study. In this work, as in others reported in the literature [34], it was supposed that both gas and liquid phases considered behave ideally. This simplification is consistent with the composition, phases and conditions of the phases here considered.

Exergy destruction (I) in a control volume is defined by [42,52]:

$$I = E_{t,in} - E_{t,out}$$

$$= \left\{ \sum_{i=1}^{N_{in}} E_{i,in} + |W_{in}| + \sum_{i=1}^{N_{Q,in}} \left[Q_i \left(1 - \frac{T_0}{T_i} \right) \right] \right\} - \left\{ \sum_{i=1}^{N_{out}} E_{i,out} + W_{out} + \sum_{i=1}^{N_{Q,out}} \left[|Q_i| \left(1 - \frac{T_0}{T_i} \right) \right] \right\}$$

(4)

where $E_{t,in}$ and $E_{t,out}$ are the total exergy of input and output streams, respectively; $E_{t,in}$ and $E_{i,out}$ are the exergy of input and output material streams (defined by equation (1)), respectively; N_{in} and N_{out} are the number of input and output material streams, respectively; $N_{Q,in}$ and $N_{Q,out}$ are the number of input and output heat streams, respectively; W_{in} and W_{out} are the total input and output work streams, respectively; and Q_i represents the heat flow to or from the control volume and T_i is the average temperature of the heat transfer fluid or media.

The exergetic efficiency (e) is defined as the ratio of total incoming exergies to total outgoing exergies. This way:

$$\varepsilon = \frac{E_{t,out}}{E_{t,in}}$$

(5)

Other definition for exergetic definition of a control volume or equipment, which is called rational exergetic efficiency, is made of the ratio of the desired exergy output from the control volume or equipment and the exergy input to the control volume or equipment [6,37]. This way [42]:

$$\varepsilon = \frac{|\Delta E_{desired}|}{|\Delta E_{desired}| + I}$$

(6)

where $|\Delta E_{desired}|$ is the variation of exergy. **Table S2** lists the equations used for computing the exergy efficiencies of all the equipment used in this work, which have been reported elsewhere [37].

3. Computational details

Aspen HYSYS V14 was used as the reference simulator in this study. Converged process flow diagrams (PFD) were defined for each example. Process variables such as the molar or mass flow rates, pressure, vapour fraction and temperature can be exported or imported respectively from or to Aspen HYSYS to MS Excel VBA, respectively, via object linking and embedded (OLE) automation. Likewise, thermodynamic variables as molar or mass enthalpy or entropy can be imported from the simulator to MS Excel VBA. The VBA codes controlled the process and performed all external computations taking the information obtained from Aspen HYSYS. Obviously, the results of these computations can be exported to the simulator. In a previous work, more information about the way to make the automation process was described in detail [53]. **Table 1** shows the way in which MS Excel assign some process variables of a hypothetical stream S1 to a hypothetical variable A.

Taking as a reference the process variables evaluated by Aspen HYSYS, the physical exergy of a hypothetical material stream A defined by equation (2) can be computed by the simulator as:

$$\begin{pmatrix} \textbf{Physical exergy} \\ \textbf{of Stream A} \end{pmatrix} = \begin{pmatrix} \textbf{Mass flow} \\ \textbf{of Stream A} \end{pmatrix} \left[\begin{pmatrix} \textbf{Mass enthalpy} \\ \textbf{of Stream A} \end{pmatrix} - \begin{pmatrix} \textbf{Temperature of} \\ \textbf{the environment} \end{pmatrix} \begin{pmatrix} \textbf{Mass entropy} \\ \textbf{of Stream A} \end{pmatrix} \right]$$

(7)

Physical exergy associated to a hypothetical heat or work stream B can be computed as follows [52]:

$$\begin{pmatrix} \textbf{Physical exergy} \\ \textbf{of the energy stream B} \end{pmatrix} = \begin{cases} \textbf{Heat: } Q_B \left(1 - \frac{T_0}{T_B} \right) \\ \textbf{Work: } W_B \end{cases}$$

(8)

Table 1. Objects used by MS Excel VBA to assign values to a process variable object in Aspen HYSYS.

Process variable	Assign an object to a variable
Temperature of stream S1	A= hyStreams.Item("S1").TemperatureValue
Pressure of stream S1	A= hyStreams.Item("S1").PressureValue
Vapour Fraction of stream S1	A= hyStreams.Item("S1").VapourFractionValue
Molar fraction of Methane in stream S1	A=hyStreams.Item("S1").ComponentMolarFractionValue("Methane")
Mass flow of stream S1	A= hyStreams.Item("S1").MassFlowValue
Molar flow of stream S1	A= hyStreams.Item("S1").MolarFlowValue
Mass enthalpy of stream S1	A= hyStreams.Item("S1").MassEnthalpyValue
Mass entropy of stream S1	A= hyStreams.Item("S1").MassEntropyValue

In this work, an average temperature of the heat transfer fluids in the different examples was considered. This is a typical approach in preliminary or conceptual process design.

The computation of the chemical exergy is a little bit more complicated since component molar or mass fractions and molar or mass component flows cannot be exported to Aspen HYSYS. A simple solution is to add to the main flowsheet to be analysed an independent part which includes the same number of streams as that of components. These streams, which are at atmospheric conditions and have an initial molar flow of 1 kmol/h, are constituted by pure components. They are named to as the prefix REF plus the name of the component in the Aspen HYSYS database. During the evaluation of the chemical exergies of all the streams present in the flowsheet, the total molar of flow of the REFcomponent streams were fixed at the same values of the corresponding component molar flow molar of the component in the stream to be analysed. All these streams enter in a mixer (REFM1). The outlet stream from the mixer (REF FROM REFM) is conducted to a heater (REF-COOLER). The temperature and pressure of the outlet stream of this block (REFTOREFF) was fixed at 293.15 K and 1 atm (environment conditions). It has been observed that even in mixtures of very similar components the mixing heat slightly alters the temperature of the resulting stream. REFTOR-EFF could be constituted by two phases (vapour and liquid). These phases will be separated in REFSEP. The molar or mass flow and molar fraction composition of the resulting streams REFV (vapour) and REFL (liquid) together with the tabulated values of the molar chemical exergy of each involved specie in both phases at T_0 and P_0 [51] would allow to evaluate, through equation (3), the chemical exergy of a specific stream which is represented by stream REF-PROD. In the bottom part of **Figure 1**, the part of the flowsheet described above is shown. Similar strategy was used for the rest of cases considered.

Figure S1 shows some sheets of the MS Excel application able to connect VBA code to Aspen HYSYS files, extract information from them and process it to compute the physical, chemical, and total exergies, and the exergetic efficiencies for each block.

Next, a set of cases that demonstrate the methodology here proposed will be presented. They allow to compute the exergies of single streams, and perform exergy analysis of a CO_2 mixer, a cooler, a distillation column, a reactor, different configurations of separating components by distillation, and a multiple recirculation process.

4. Results and discussion

4.1 Case 1: Exergies of single streams

Two cases, corresponding to two streams (Stream 1 and Stream 2) were here considered which were taken from the literature [42]. Similarly, SRK was the fluid package chosen for both cases. They were selected to validate the methodology here proposed. The conditions required to complete the simulation are listed in **Figure 1** and **Figure 2**. **Table 2** lists the values of the total exergy and its constituent parts for Stream 1 and Stream 2 computed by the methodology proposed in this work and that evaluated by Abdollahi-Demneh et al. The former were obtained with Aspen HYSYS V14 whereas the latter were obtained with Aspen HYSYS release corresponding to the year of the paper publication (2011). Similar results were obtained in both cases. Since it is expected that the physical exergy computed with both releases should be very similar, it seems that the temperature and pressure of Stream 2 reported by these authors should be slightly different to that used in the simulator.

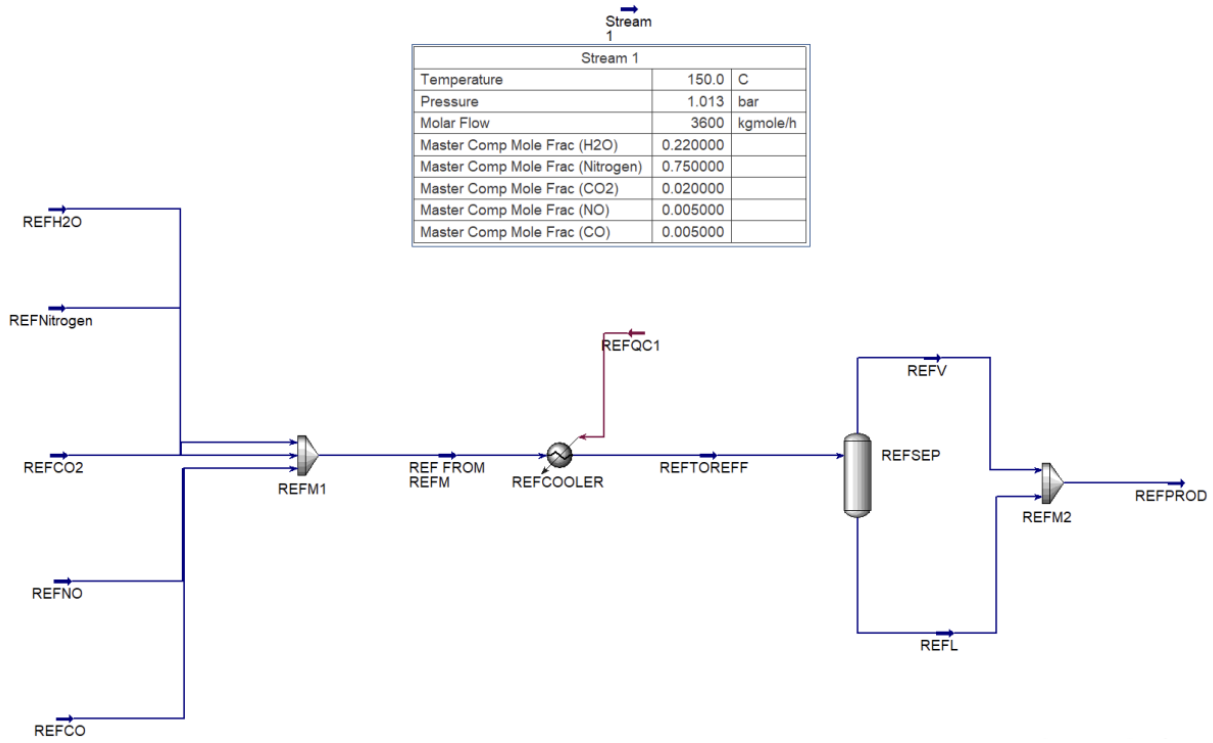This simple methodology was extended to other cases.

Figure 1. Flowsheet of Case 1: exergy of Stream 1.
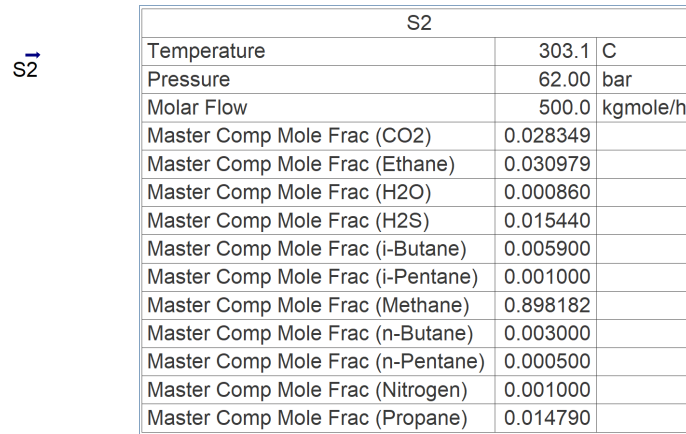
Source: Abdollahi-Demneh [42].

Figure 2. Flowsheet of Case 1: exergy of Stream 2.

Source: Abdollahi-Demneh [42].

Table 2. Total exergy and its constituent parts for Stream 1 and Stream 2. Comparison with the results reported in the literature.

Stream	Methodology	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Stream 1	[42]	1287.4	2446.3	3733.7
	This work	1288.1	2514.4	3802.5
Stream 2	[42]	1376.5	118437.1	119813.6
	This work	1942.8	120770.8	122713.6

Source: Abdollahi-Demneh [42].

4.2 Case 2: Exergy analysis of a CO_2 mixer

Figure 3 shows the simulation of a CO_2 mixer constituted by two entering streams resulting in just one. One of the streams (CO2AP) suffers a decompression to get the same pressure of Stream CO2BP. Data for completing the simulations are included in the figure. Peng Robinson was chosen as the Fluid Package. This process does not lead a change of chemical exergy since neither reaction or separation were involved. **Table 3** lists the total exergy and its constituent parts for the streams involved in Case 2. In the same table, the exergy destruction of the whole process and the exergetic efficiency is also shown. As expected, the presence of a valve leading to the expansion of Stream CO2AP caused the major part of the loss of work of the process, which was estimated in 0.52 kW (80% of the total exergy destruc-

tion of the process).

4.3 Case 3: Exergy analysis of a cooler

Figure 4 shows the simulation of a cooler constituted by an inlet and an outlet material streams, and an outlet energy stream. Similarly to previous cases, data for completing the simulations are included in the figure. In this case, Peng Robinson was chosen as the Fluid Package. This process does not lead to a change of chemical exergy regardless any reaction or separation is involved. **Table 4** lists the total exergy, its constituent parts for the streams involved in Case 2 and the corresponding exergetic efficiency (**Table S2**). By assuming that the temperature of the cooling media was 10 ºC lower than that of Stream OUT (142.3 ºC), equation (8) was used for computing the physical exergy of energy Stream Q.
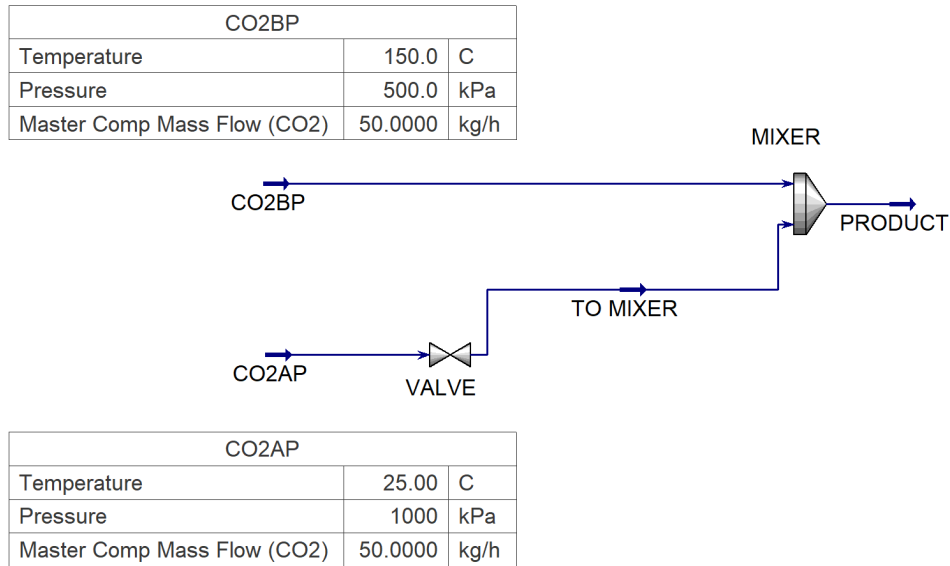
CO2BP		
Temperature	150.0	C
Pressure	500.0	kPa
Master Comp Mass Flow (CO2)	50.0000	kg/h

CO2AP		
Temperature	25.00	C
Pressure	1000	kPa
Master Comp Mass Flow (CO2)	50.0000	kg/h

Figure 3. Flowsheet of Case 2: exergy analysis of a CO_2 mixer.

Table 3. Total exergy and its constituent parts for the streams involved in Case 2: exergy analysis of a CO_2 mixer. Exergy destruction (equation 4) and exergetic efficiency (equation 5) of the whole process.

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
CO2BP	1.501	6.271	7.772
CO2AP	1.752	6.271	8.023
TO MIXER	1.232	6.271	7.503
PRODUCT	2.603	12.541	15.145
		Exergy destruction (I) (kW)	0.650
		Exergetic efficiency (ε)	0.959

The use of the corresponding equation in **Table S2** leads to a value of exergetic efficiency slightly higher than 1, because of the values stored in the simulator, when that computed from equation (6) is lower than 1. The latter represents more clearly the real situation of the process.

An additional issue would be the influence of the pressure drop in the cooler on the exergy destruction and the different definitions of the exergetic efficiency. Thus, by considering a value of the pressure drop of 1 bar the expected following values would be obtained: exergy destruction: 1.015 kW; exergetic efficiency computed by equation (6): 0.953; and exergetic efficiency by the corresponding equation in **Table S2**: 1.059.
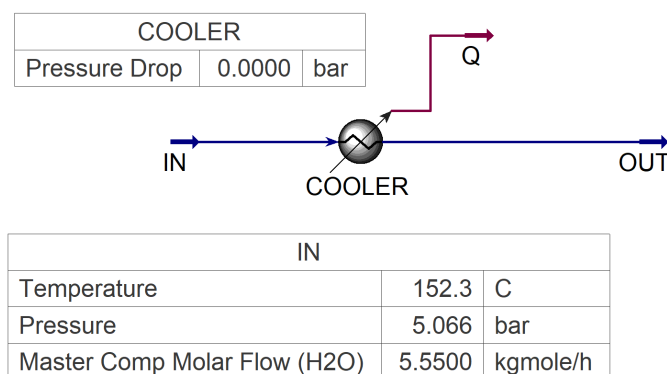
COOLER		
Pressure Drop	0.0000	bar

Q

IN   OUT
COOLER

IN		
Temperature	152.3	C
Pressure	5.066	bar
Master Comp Molar Flow (H2O)	5.5500	kgmole/h

Figure 4. Flowsheet of Case 3: exergy analysis of a cooler**.**

Table 4. Total exergy and its constituent parts for the streams involved in Case 3: exergy analysis of a cooler. Exergy destruction (equation 4) and exergetic efficiency (equation (6) and the corresponding equation in **Table S2**) of the whole process.

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
IN	20.331	1.388	21.719
OUT	2.637	1.388	4.025
Q	16.692	-	16.692
		Exergy destruction (I) (kW)	1.002
		Exergetic efficiency (ε) equation (6)	0.954
		Exergetic efficiency (ε) (*Table S2*)	1.060

4.4 Case 4: Exergy analysis of distillation column

Figure 5 shows the simulation of a distillation column. It includes all the information for converging the simulation. Peng Robinson was chosen as the Fluid Package. Unless the previous cases, this one leads to a change of chemical exergy of the material streams since a separation of components is involved. **Table 5** lists the total exergy, its constituent parts for the streams involved in Case 4 and the corresponding exergetic efficiency (**Table S2**). By assuming that the temperature of the cooling media in the condenser was 10 ºC lower than that of Stream D (–21.8 ºC) and that of the heating media in the reboiler was 10 ºC higher than that of Stream B (88.3 ºC), equation (8) was used for computing the physical exergy of energy the streams Q_D and Q_B.

The use of equation (9) leads to a value of exergetic efficiency very low and negative, which means that the process is not very efficient according to the criteria proposed. Negative values of exergetic efficiencies have reported in literature [52]. The exergetic efficiency computed by equation (6) is, as expected, lower than 1.
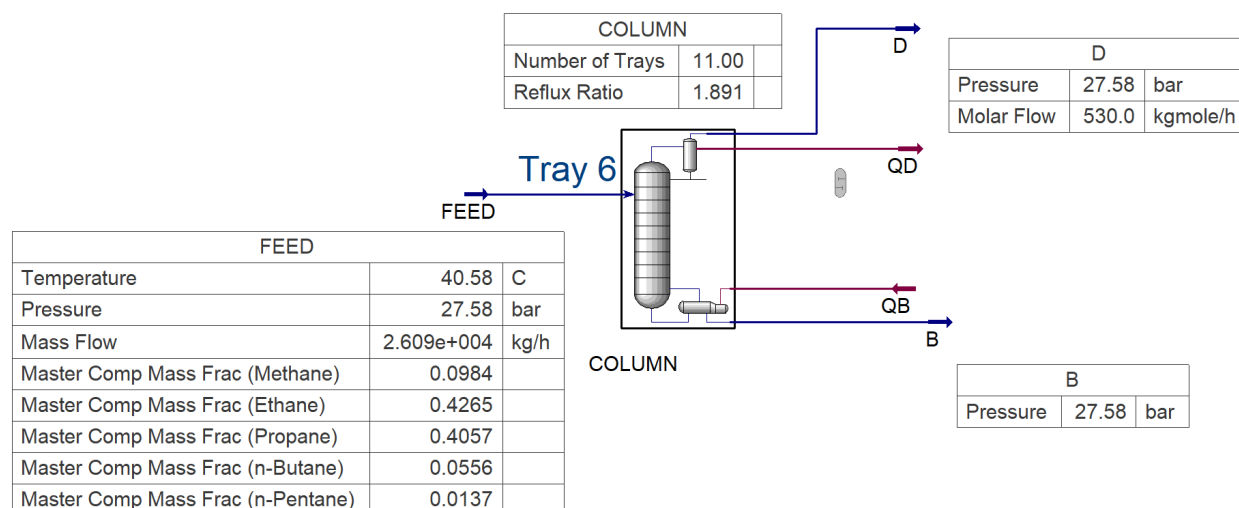
Figure 5. Flowsheet of Case 4: exergy analysis of a distillation column.

Table 5. Total exergy and its constituent parts for the streams involved in Case 4: exergy analysis of a distillation column. Exergy destruction (equation 4) and exergetic efficiency (equation (6) and the corresponding equation in **Table S2**) of the whole process.

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
FEED	1677.8	362408.5	364086.3
D	1159–443	193302.4	194461.9
B	426.1	169371.8	169797.9
Q_B	333.5		333.5
Q_D	−533.7		−533.7
		Exergy destruction (I) (kW)	693.7
		Exergetic efficiency (ε) equation (6)	0.998
		Exergetic efficiency (ε) (Table S2)	−1.080

4.5 Case 5: Exergy analysis of a reactor

Figure 6 shows the simulation of a reactor where the exothermic reaction of hydrogenation of aniline to yield cyclohexylamine whose data were taken from the literature [54]. NRTL-SRK was chosen as the Fluid Package. The system is constituted by two inlet material streams and an energy stream. Two outlet material streams are considered for the gas and liquid products. Process data required for simulating the process are listed in the figure. The reaction rate used in this case is as follows:

$$r\left(\frac{lbmol}{ft^3h}\right) = 10^8 exp\left[-\frac{46520\left(\frac{kJ}{kmol}\right)}{RT}\right]C_{Aniline}C_{H_2}$$

(9)

where molar concentration is expressed in lbmol/ft³.

In this case, a change of chemical exergy is expected since a chemical reaction proceeds.

Table 6 lists the total exergy, its constituent parts for the streams involved in Case 5 and the corresponding exergetic efficiency (**Table S2**). By assuming that the temperature of the cooling media was 15 ºC lower than that of the temperature inside the reactor (106.1 ºC), equation (8) was again used for computing the physical exergy of energy Stream Q. The use of the corresponding equation in **Table S2** leads to a value of exergetic efficiency close to 1. This value is slightly higher than that computed by equation (6).
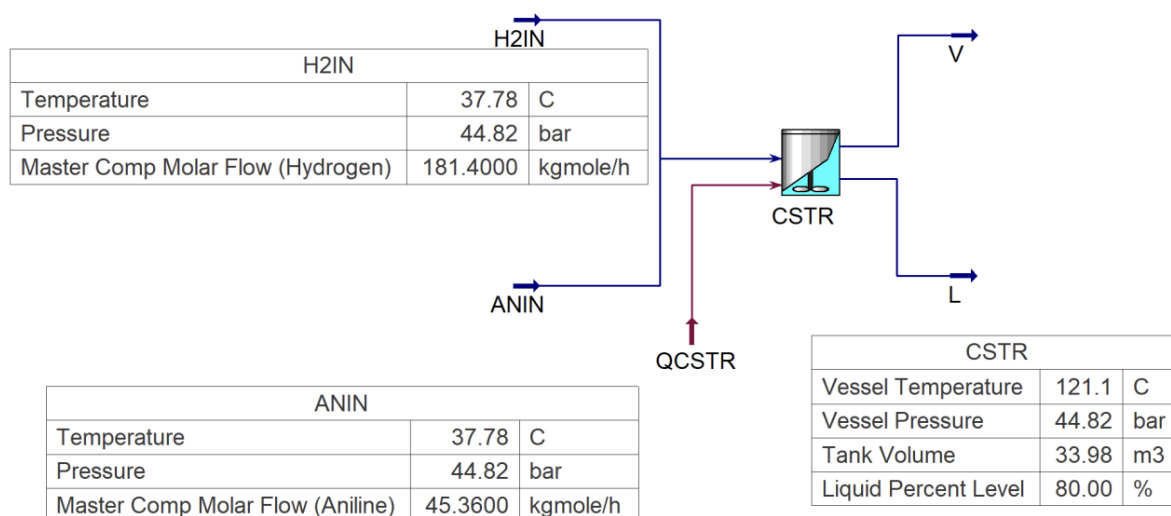
Figure 6. Flowsheet of Case 5: exergy analysis of a reactor.

Table 6. Total exergy and its constituent parts for the streams involved in Case 5: exergy analysis of a reactor. Exergy destruction (equation 4) and exergetic efficiency (equation (6) and the corresponding equation in **Table S2**) of the whole process.

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
H2IN	477.4	11896.8	12374.2
ANIN	44.6	42298.8	43443.4
V	214.7	6277.3	6492.1
L	20.0	48978.5	48998.5
QCSTR	318.5		318.5
		Exergy destruction (I) (kW)	8.6
		Exergetic efficiency (ε) equation (6)	0.999
		Exergetic efficiency (ε) (Table S2)	0.974

4.6 Case 6: Exergy analysis of a multiple recirculation process

Figure 7 shows the simulation of a multiple recirculation process (natural gas compression) which appeared in former Operation Guides and Tutorials of HYSYS. In this case, Peng-Robinson was used as the Fluid Package. Pressure drop in all the coolers was set to 5 psi. Temperature of the outlet stream was fixed at 48.9 ℃ and the pressure of coolers E-100, E-101 and E-102 were fixed at 1379, 3447 and 6895 kPa, respectively. This process also causes a change of chemical exergy of the streams since separation processes are involved. **Table 7** also lists the total exergy, its constituent parts for the streams

involved in Case 6 and the corresponding exergetic efficiency (**Table S2**). In this case, the temperatures of the cooling were 15 ℃ lower than that of the corresponding outlet stream from the coolers. Exergy destruction was computed with equation (6).

On the other hand, **Table 8** lists the exergy efficiency of all the blocks computed according to equations shown in **Table S2**. As expected, the lowest values of efficiency were obtained with compressors and coolers. Finally, **Figure 8** plots the influence of difference of temperature between the cooling media and the outlet streams of all the coolers on the exergy destruction: the lower the difference, the lower the value of exergy destruction was.

Table 7. Total exergy and its constituent parts for the streams involved in Case 6: exergy analysis of a multiple recirculation process. Exergy destruction (equation 4) of the whole process.

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
FEED	1195.8	573205.4	574401.1
V-103 VAP	2298.6	303273.5	305572.1
V-100 LIQ	49.4	267608.5	267657.9
K-100 DUTY	749.0		749.0
K-101 DUTY	799.0		799.0
K-102 DUTY	555.2		555.2
E-100 DUTY	11.0		11.0
E-101 DUTY	31.3		31.3
E-102 DUTY	34.0		34.0
		Exergy destruction (I) (kW)	3198.1
		Exergetic efficiency (ε)	0.994

Table 8. Exergy efficiency of all the equipment in Case 6 computed according to **Table S2**.

Block	Type of equipment	Exergy efficiency	Block	Type of equipment	Exergy efficiency
MIX-100	Mixer	1.000	K-101	Compressor	0.797
V-100	Separator	0.997	E-101	Cooler	0.234
K-100	Compressor	0.781	MIX-102	Mixer	1.000
E-100	Cooler	0.216	V-102	Separator	1.000
MIX-101	Mixer	1.000	K-100	Compressor	0.798
V-101	Separator	0.999	E-102	Cooler	0.236
			V-103	Separator	1.000

Source: Ghannadzadeh [37].
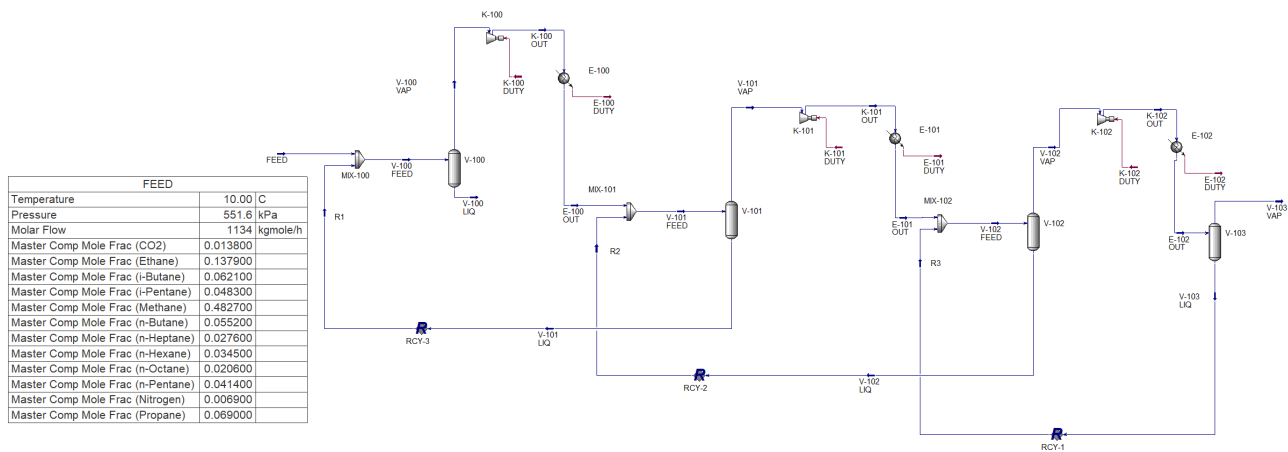
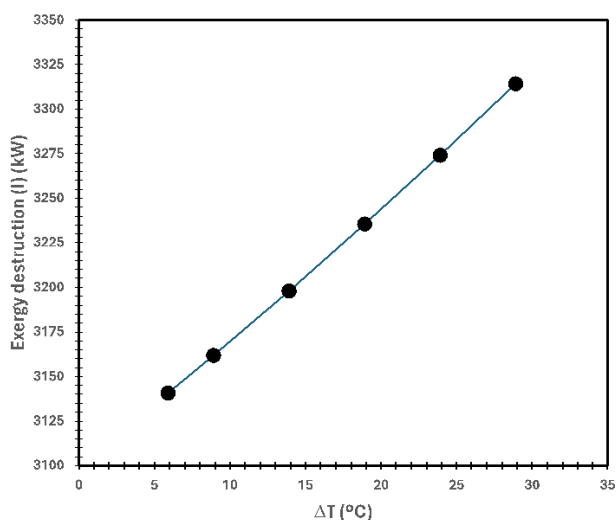**Figure 7.** Flowsheet of Case 6: exergy analysis of a multiple recirculation process.

Figure 8. Flowsheet of Case 6: multiple recirculation process. Influence of difference of temperature between the cooling media and the outlet streams of all the coolers on the exergy destruction.

4.7 Case 7: Exergy analysis of different configurations of separating components by distillation

Recently, five structures for gas condensate stabilization were simulated using Aspen HYSYS and analysed from the energy, exergy, economic and environmental points of view [55]. Peng Robinson was chosen as the Fluid Package. The studied structures are a stabilizer column with reboiler and condenser and without preheating (Stabilizer 1), a stabilizer column with reboiler, without condenser and with preheating (Stabilizer 2), a stabilizer column with reboiler and without condenser (Stabilizer 3), a stabilizer column with reboiler, condenser and preheater (Stabilizer 4), and a stabilizer column with reboiler, without condenser and with side reboiler (Stabilizer 5). **Figure 9** shows the flowsheet with all the structures considered and data to complete the feed whereas **Table S3** lists the rest of data to complete the simulation. This process also leads to a change of chemical exergy of the streams since separation processes are involved. Unlike this work, Matsui and Le just considered the physical exergy instead of both physical and chemical exergies. **Table 9** lists the total exergy and its constituent parts for the five scenarios considered in Case 7. In this case, the

temperatures of the cooling and heating media of all condensers and reboilers were 15 ºC lower and higher, respectively, than that of the corresponding outlet and inlet streams, respectively. In addition, the exergy destruction computed in this work plus that computed by Matsui and Le and the exergy efficiency evaluated with equation (6). It can be observed that the results obtained are in the same order of magnitude. As expected, the alternatives that considers energy integration led to a lesser exergy destruction. Specifically, stabilizers 2 and 4, where a heat exchange between the bottom stream from the column and the feed entering the system was located, presented the most favorable values of exergy destruction. The latter, which does not include a condenser, was the one with the lowest value of exergy destruction and hence it should be considered as the best option for stabilizing the feed.

5. Conclusions

In this work, a general procedure for computing all those physical values based on adding a simple flowsheet to the main one was designed. By additionally integrating the evaluation by the MS Excel VBA application linked to a simulation case in Aspen HYSYS of the exergy efficiencies of the different blocks in a flowsheet, the software developed was able to exergetically evaluate any process and its components. Seven cases (single streams, CO_2 mixer, cooler, distillation column, reactor, different configurations of separating components by distillation, and a multiple recirculation process) were used to present and validate a methodology for computing physical, chemical and total exergies, and the exergy destruction and the exergetic efficiency of simple and complex processes by using the object linking and embedded (OLE) automation by connecting Aspen HYSYS to MS Excel VBA. The basis of this methodology has been used for designing tools for computing exergy, exergoeconomic and exergoenvironmental analysis of chemical processes through Aspen HYSYS and Aspen Plus simulations and should be used for discriminating among different process alternatives.

Table 9. Total exergy and its constituent parts for the streams involved in Case 7: exergy analysis of different configurations of separating components by distillation. Exergy destruction (equation 4) and the corresponding equation in **Table S2** of the whole process.

STABILIZER 1

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Feed	57.2	239336.0	239393.2
Off Gas-ST1	75.5	20544.0	20619.4
St Condensate ST1	371.8	218123.9	218495.7
QD-ST1	-0.24		-0.24
QR-ST1	715.6		715.6
		Exergy destruction (I) (kW)	993.9
		Exergetic efficiency (ε) equation (6)	0.996
		Exergy destruction (I) (kW) (Table S2)	1295.0

STABILIZER 2

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Feed-2	57.2	239336.0	239393.2
St Condensate-ST2	123.7	217050.7	217174.5
Off Gas-ST2	77.0	21811.9	21888.9
QD-ST2	-2.54		-2.54
QR-ST2	455.1		455.1
		Exergy destruction (I) (kW)	787.4
		Exergetic efficiency (ε) equation (6)	0.997
		Exergy destruction (I) (kW) (Table S2)	694.5

STABILIZER 3

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Feed-3	57.2	239336.0	239393.2
Off Gas-ST3	76.4	20818.7	20895.1
St Condensate-ST3	371.3	217852.1	218223.4
QR-ST3	714.2		714.2
		Exergy destruction (I) (kW)	988.9
		Exergetic efficiency (ε) equation (6)	0.996
		Exergy destruction (I) (kW) (Table S2)	1298.0

STABILIZER 4

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Feed-4	57.2	239336.0	239393.2
Off Gas-ST4	92.8	28603.8	28696.6
St Condensate-ST4	119.0	210443.0	210562.0
QR-ST4	433.6		433.6
		Exergy destruction (I) (kW)	568.2
		Exergetic efficiency (ε) equation (6)	0.998
		Exergy destruction (I) (kW) (Table S2)	717.8

STABILIZER 5

Stream	Physical Exergy (kW)	Chemical Exergy (kW)	Total Exergy (kW)
Feed-5	57.2	239336.0	239393.21
Off Gas-ST5	76.6	20956.7	21033.2
St Condensate-ST5	156.2	217681.5	217837.7
QR-ST5	452.6		452.6
		Exergy destruction (I) (kW)	974.9
		Exergetic efficiency (ε) equation (6)	0.996
		Exergy destruction (I) (kW) (Table S2)	681.9

Figure 9. Flowsheet of Case 7: exergy analysis of different configurations of separating components by distillation.

Authors Contributions

This work was done jointly by all authors. Jose Luis Valverde developed the code on Microsoft Office Excel. Victor Ferro and Loredana Postolache chose for and prepared the simulations. Anne Giroir-Fendler supervised the results obtained. Anne Giroir-Fendler and Loredana Postolache worked on the data interpretation and result discussion. Víctor Ferro and Jose Luis Valverde coordinated the whole study, the manuscript review and revision.

Conflict of Interests

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Data Availability Statement

The authors declared that the simulations and the spreadsheets used are available for anyone interested on them.

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Appendix

Table S1. Values of the molar chemical exergy of all the species considered in this study [1].

Specie name (Aspen HYSYS)	$(b_i^0)_{vapour}$ (kJ/mol)	$(b_i^0)_{liquid}$ (kJ/mol)
H_2O	9.50	0.90
N_2	0.72	-
CO_2	19.87	-
NO	88.90	-
CO	275.10	-
H_2	236.10	-
H_2S	812.00	-
Methane	831.65	899.19
Ethane	1495.04	1552.49
Propane	2154.00	2207.77
i-Butane	2863.54	2863.54
n-Butane	3463.30	2863.54
i-Pentane	-	3519.51
n-Pentane	-	3475.59
n-Heptane	-	4114.50
n-Octane	-	4761.70
n-Nonane	-	6064.90
n-Decane	-	6716.00
n-C11	-	7376.00
n-C12	-	8029.40
M-Mercaptane	-	1826.23
E-Mercaptane	-	2500.37
diM-Sulfide	-	2500.37
Aniline	-	3444.35
CC6Amine	-	4150.60

Table S2. Exergy efficiencies of all the equipment used in this work [2].

Equipment	Exergy efficiency
Compressor	$\dfrac{B_{out} - B_{in}}{B_{shaftwork}}$
Heater	$\dfrac{B_{out} - B_{in}}{B_Q}$
Cooler	$\dfrac{B_{in} - B_{out}}{B_Q}$
Exothermic reactor	$\dfrac{B_{in} - B_{out}}{B_Q}$
Separator	$\dfrac{\sum B_{out}}{B_{in}}$
Mixer	$\dfrac{B_{out}}{\sum B_{in}}$
Distillation column	$\dfrac{B_D + B_B - B_{feed} + B_{Q_D}}{B_{Q_B}}$

Table S3. Extra data required in Case 6 for completing the degrees of freedom of the flowsheet and performing the exergy analysis.

Stream	Variable	Value	Block	Variable	Value
Off Gas-ST1	Temperature	35 ℃	Stabilizer 1	Number of stages	15
St Condensate- ST1	RVP ASTM D323-73/79	8 psia	Stabilizer 1	Feed stage	1
Feed-2 to S2	Temperature	90 ℃	Stabilizer 1	Type of condenser	Partial
R ST2	RVP ASTM D323-73/79	8 psia	Stabilizer 2	Number of stages	15
St Condensate-ST3	RVP ASTM D323-73/79	8 psia	Stabilizer 2	Feed stage	1
Feed4 to S4	Temperature	90 ℃	Stabilizer 2	Type of condenser	Partial
R ST4	RVP ASTM D323-73/79	8 psia	Stabilizer 3	Number of stages	15
St Condensate-ST3-2	RVP ASTM D323-73/79	8 psia	Stabilizer 3	Feed stage	Top
St Condensate-ST5	Temperature	123.4 ℃	Stabilizer 4	Number of stages	15
			Stabilizer 4	Feed stage	Top
			Stabilizer 5	Number of stages	15
			Stabilizer 5	Feed stage	Top
			Stabilizer 5	Side draw stage	8 (liquid)
			Stabilizer 5	Stage 4 temperature	119.8 ℃
			Stabilizer 5	Side draw rate	200 kmol/h

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Figure S1. Sheets of the ExH application able to process Aspen HYSYS simulation cases to evaluate total, physical and chemical exergies.

Source: Ghannadzadeh [37] and Szargut [51].