

Review Article

Automation of Process Simulations with Aspen Plus

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Introduction

The use of process simulation software has had great impact on the chemical engineering curricula during the last years [6]. They are a valuable tool not only for process design, but also for process optimization, tuning of the control loops or training of operators [19]. To make an effective use of the simulators, process engineers must know the performance of the models provided by each simulator (Gil Chaves et al., 2016). Sometimes they often find limitations when designing their own applications or experiments [5]. A solution is to automate the simulation process with third party software [13]. Automation permits programmers to run objects within a program which could be used by other ones. Several examples have been reported in the literature of using different applications or programming languages (Matlab, Python, MS Excel-VBA, C++, etc.) linked to commercial simulators like Aspen HYSYS [1,2,8,11,13,14,18,19, 21,23,24,25,28], Aspen Plus [15,22,25,26] and UNISIM [9].

The use of Automation can help students to understand concepts as that of the multi-disciplinary analysis optimization (MDAO) tools, which was introduced by NASA (<https://software.nasa.gov/software/LEW-18550-1>) and consists of the development of a "central executive" computational unit capable of communicating with external analysis tools and collect the information needed for the optimization design. These tools are typically developed as a single large software application that performs analysis for all disciplines but has little or no capability

Abstract

Automation of commercial simulation software to third-party applications allow to connect different software around a central model which would improve their ability to optimize and operate productive processes. In this work, three production processes taken from literature, have been proposed to demonstrate the capability of the Automation concept by using Aspen Plus: the cyclohexane production from benzene and the production of biphenyl (sensitivity analysis), 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-. The way in which the different cases are raised and the solutions are extensively discussed.

Keywords: Automation; Aspen plus; MS Excel-VBA; Chemical process

ity to integrate different components that have already been developed as stand-alone analysis codes [7].

Currently, automation gains and even will gain more importance due to the increasing role of the artificial intelligence in process engineering, the control of plant operations and the end-to-end regulation and optimization of the processes. This phenomenon, among other features, includes the creation of extended nets of liked software around a central model. The formers fulfill specific functions related to the data collection and analysis, process and operations optimization and control, the interconnection of all the organizations involved in the productive process, etc. Among the programs to be used in the process and operations optimization and control, commercial process simulators are a confident option. Thus, they must be interconnected via automation with all the remainder infrastructure of the process digital twin. To successfully face this reality during their working life, the chemical engineering's students need to acquire knowledge and skills in the automation of commercial process simulators with third party software as those already mention here. Unfortunately, these themes not always are included in the current curricula of the Chemical Engineering Bachelors and Masters. By this reason, the option to include them through short courses, seminars, etc. seams to be an adequate alternative.

In a recent paper, Santos and Van Gerven [19] studied the connection methodologies of the popular 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. In other recent paper, the values of the binary interaction parameters of the e-NRTL model for different salts in water included in the Aspen Plus database were refined [24]. The e-NRTL equation was solved by using a procedure implemented in Aspen Plus by linking the process simulator and the MS Excel VBA code via Automation as the third-party software [25].

In a recent paper, the capability of Automation as a powerful tool for simulating unprecedented complex processes was demonstrated in a seminar by combining the commercial simulator Aspen-HYSYS and MS Excel-VBA [24]. Although the Automation processes conducted with Aspen Plus and Aspen HYSYS are conceptually similar, they are methodologically very different as it can be checked by comparing the results of this work with those reported in the above-mentioned previous paper. Three study cases were considered: the cyclohexane production from benzene and the production of biphenyl [20], the optimization without constraints of the composition of a stream from the production of cumene, whose data were taken from the course of introduction to Aspen Plus performed by Aspen Technology Inc., and the optimization with constraints of the isomerization of nC_4 - to iC_4 - which was developed through information reported elsewhere [3,12,16,17,27].

Theory (Computational details)

Aspen Plus V12.1 was employed in this study as the reference simulator. Converged Process Flow Diagrams (PFD) were defined for each of the examples considered. Process variables used in the different computations were imported or exported from Aspen Plus to MS Excel-VBA and vice versa via Object Linking and Embedded (OLE) Automation. VBA codes controlled the process and performed all the external computations out of Aspen Plus. Although the Automation concept was applied in the same way for both cases of study, the strategies followed for reaching the solution demanded by each one were different.

The allocation of any variable in Aspen Plus to be linked to MS Excel-VBA is easy to get from the *Customize Tab* by clicking on *Variable Explorer*. For example, if the temperature (input variable) of a given stream S1 must be located, one must consecutively click on Root-Data-Streams-S1-TEMP-MIXED (Figure 1). This way, the following instruction should be located on the VBA code:

```
Application.Tree.FindNode("\Data\Streams\S1\Input\TEMP\MIXED")
```

Where Application represents the name of the application object created by the user. To assign a value to this variable or read the value contained in, the instruction must contain as an append the text "Value". Thus, if the application object is named to as "ihAPsim" the following instructions are possible:

```
ihAPsim.Tree.FindNode("\Data\Streams\S1\Input\TEMP\MIXED").Value = 200
```

```
TS1 = ihAPsim.Tree.FindNode("\Data\Streams\S1\Input\TEMP\MIXED").Value
```

When an application is exposed for Automation, a separate file is usually created that lists all the objects and their respec-

tive properties and methods. In this case, the file Aspen Plus GUI 39.0 Type Library must be selected. For this purpose, one must go to the References command in the VBA Tools Menu, check the box next to the above-mentioned file and then click the OK button.

Results and Discussion

Case of Study 1: Production of Cyclohexane from Benzene

Figure 2 shows the process flowsheet considered in this study. The aim of this example was to analyze different scenarios where the reactor duty and the composition of hydrogen and cyclohexane in two product streams were computed as a function of the benzene conversion in the reactor. The variables listed in the flowsheet allow converging the case and were taken from the literature [20].

The block diagram used for designing the MS Excel-VBA application is shown in Figure 3. An Excel file template which allows building the final application can be used (Figure S1). A sheet is defined: COMPUTATIONS, where the scenarios to be analysed and view the results can be introduced. The name and allocation of the Aspen Plus file used in the Automation process should be introduced before proceeding with the simulation (.bkp extension). Regarding the block diagram, a unique module is defined where the main processes of clearing cells, reading the Aspen Plus file and making the Automation are performed.

The instructions included in this module are the following ones:

File name reading and creation of the application object:

```
FASP = Cells (3, 2)
```

```
Set ihAPsim = GetObject (FASP, "Apwn.Document.39.0")
```

```
Application.Visible = True
```

```
ihAPsim.Visible = True
```

```
Do-While structure for reading all data supplied by user:
```

```
I = 1
```

```
Do While Cells (5 + I, 1) <> ""
```

```
Conversion of benzene is read:
```

```
ihAPsim.Tree.FindNode("\Data\Blocks\R1\Input\CONV\1").Value = Cells(5 + I, 1)
```

Aspen Plus is forced to run and wait for 2 seconds; this time is required for completing the new simulation:

```
ihAPsim.RUN
```

```
Application.Wait (Now + TimeValue("00:00:02"))
```

Reactor duty, composition of H_2 in S11 and cyclohexane in S16:

```
Cells (5+I, 2) = ihAPsim.Tree.FindNode("\Data\Blocks\R1\Output\QCALC").Value
Cells (5+I, 3) = ihAPsim.Tree.FindNode("\Data\Streams\S11\Output\MOLEFRAC\MIXED\H2").Value
Cells (5+I, 4) = ihAPsim.Tree.FindNode("\Data\Streams\S16\Output\MOLEFRAC\MIXED\CYCLOHEX").Value
```

```
Update of the counter and end of the Do-While Structure:
```

```
I = I + 1
```

Loop

Units of the variables transferred are equal to those defined in the Aspen Plus file.

Figure S2 shows the complete VBA code but that of the buttons. Finally, Figure 4 shows the results obtained from the Aspen Plus interaction.

Case of Study 2: Optimization without constraints of the composition of a stream from the production of cumene

The corresponding Aspen Plus diagram is shown in Figure 5. The aim of this example is to compute the temperature of stream TOSEP (T_{TOSEP}) that leads to a value of molar fraction of propene (x_p) in stream L of 0.1. For this purpose, the Regula-Falsi method was used once it was verified that the searched molar fraction was in the interval 90 °C ($x_p=0.0199$) and 120 °C ($x_p=0.077$).

The block diagram used for designing the Excel-VBA application is shown in Figure 2. A file template which allows to build the final application can be also used (Figure S3). Again, a sheet is defined: COMPUTATIONS, where the objective of x_p and the values of the T_{TOSEP} that limit the root of the function to make 0 and view the results can be entered. The name and allocation of the Aspen Plus file used in the Automation process should be again introduced before proceeding with the simulation (.bkp extension). Regarding the block diagram, several modules are defined: ACCESO, where the Automation process is located, FALPOSICION, which the Regula Falsi method is executed and FUNUNA, where the function to make 0 is defined. The instructions included in these modules are listed in Figures S4 to S6. Specifically:

Module ACCESO, including the following sentences:

x_p objective reading:

```
XP=Cells(5, 2)
```

File name reading and creation of the application object and application visible when running:

```
FASP = Cells(3, 2)
```

```
Set ihAPsim = GetObject(FASP, "Apwn.Document.39.0")
```

```
ihAPsim.Visible = True
```

Initial estimations reading:

```
X0 = Cells(8, 2): X1 = Cells(9, 2)
```

Computing objective function at the initial estimations:

```
ihAPsim.Tree.FindNode("\Data\Streams\L\Output\MOLEFRAC\MIXED\PROPENE").Value
```

```
Cells(8, 4) = XPCALC
```

```
ihAPsim.Tree.FindNode("\Data\Blocks\COOLER\Input\TEMP").Value = X1
```

```
ihAPsim.RUN
```

```
RUN
```

```
Application.Wait (Now + TimeValue("00:00:02"))
```

```
XPCALC = ihAPsim.Tree.FindNode("\Data\Streams\L\Output\MOLEFRAC\MIXED\PROPENE").Value
```

```
Cells(9, 4) = XPCALC
```

Call to Regula Falsi procedure:

```
Call FALPOS(X0, X1, FF, XX, ICON)
```

On-screen computer output:

```
Cells(11, 2) = XX: Cells(11, 4) = XPCALC
```

```
Cells(12, 2) = FF: Cells(12, 4) = ICON
```

Module FUNUNA, including the following sentences:

The value to be optimized by Regula-Falsi method is updated:

```
ihAPsim.Tree.FindNode("\Data\Blocks\SPLIT\Input\FRAC\C").Value = X
```

Aspen Plus is forced to run and wait for 2 seconds; this time is required for completing the new simulation:

```
ihAPsim.RUN
```

```
Application.Wait (Now + TimeValue("00:00:02"))
```

The temperature of stream A computed by the application is collected in Farenheit degrees:

```
XPCALC = ihAPsim.Tree.FindNode("\Data\Streams\L\Output\MOLEFRAC\MIXED\PROPENE").Value
```

The function to make 0 (F) is computed, where TA is the objective temperature (1100 °F)

```
F = XP - XPCALC ' FUNCTION TO MAKE 0
```

Finally, Figure 6 show the results obtained from the Aspen Plus interaction. As observed, the value of the T_{TOSEP} that led to a value of x_p equal to 0.01 resulted to be 11.8 °C. The result was obtained after 7 iterations.

Case of Study 3: Optimization with constraints of the isomerization of nC_4 to iC_4 .

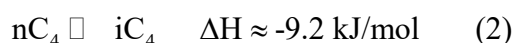
In the early stages of the process engineering (conceptual design, for example) is desirable using simplified (shortcut) models in the corresponding process simulations to avoid convergence problems and the necessity of large specification schemes when not enough information on the process is available. However, simplified models are limited by nature, being unable to reflect most of the complex relationships characteristic of the "real" systems. This is the case, for example, of the RSTOIC model for the reactors where the fractional conversion can be expressed only as function of the temperature. In several processes, nevertheless, the conversion can be also dependent on the pressure and/or the reacting mixture composition. The equilibrium-based models can consider these relationships, but the quality of the equilibrium constant computing strongly depend on the standard free energies of the components stored in the program databases.

The RSTOIC model could rigorously solve the mass balance in the reactor if the specified fractional conversion considers all the conditioning factors mentioned above. To do that, fractional conversion (X) can be computed by an equation like (1), implemented as a user model in an external program (in form of a VBA code, for example) and exported via automation to the RSTOIC model specification in Aspen Plus.

$$X = f(p, T, x_i, \dots) \quad (1)$$

where: p and T are, respectively, the operating pressure and temperature at the reactor, and x_i is the composition of the reacting mixture given as molar fraction, for example. The eq. (1) can take the form of a parametric relationship, the adjustable parameters of which are obtained by regression of experimental data. The required adjust can also be done by an external program.

The next one could be a good example of this strategy. In alkylation production processes, streams rich in isobutane (iC_4 -) are required as raw material. However, the butane's streams, usually available in refinery (Table 1SM), do not satisfy the required iC_4 - concentration for feeding the alkylation reactor. Thus, the mixed butane's streams are conveniently treated for obtaining the iC_4 - enriched stream. To achieve that, the isomerization of normal butane (nC_4 -) is carried out following the reaction described by eq. (2).



Highly active catalysts have been developed for this reaction [27] thus it takes place "very near" to the equilibrium conditions. This way, its conversion is higher for relatively low both operating temperature and iC_4 - concentration in the feed mixture to the reactor. To ensure the appropriate low iC_4 - concentration in the isomerization reactor inlet stream, the butanes mixture is treated by rectification prior to be feed to the isomerization reactor.

The Butamer process developed by the UOP (Figure S7), for example, is a solidly established technology to transform the typical refinery butane's feedstocks (Table 1S) in reach iC_4 - containing mixtures for the alkylation process [3,12,16,17,27]. Other alternatives to the same process have been developed by ABB Lummus Global, BP, etc. The process, in general, is very flexible as evidenced by the two configurations shown in Figure S7. In the industrial process, hydrogen and chloride containing organic components are added before the isomerization reactor both to improve the catalyst activity and to avoid the polymerization of the unsaturated components present in the mixture fed to the reactor and the olefin intermediates from the isomerization reaction. With the same aim, reaction temperature is maintained as low as possible. For simplicity, in the current example, the hydrogen and chloride additions are omitted and the alternative having only the deisobutanizer column is considered (Figure 7S).

Isomerization reactor operates at temperatures and pressures in the intervals between 145 - 220°C and 15 - 30 bar, respectively. Under these conditions, the nC_4 - to iC_4 - conversion per pass reached is about 50-60% being the selectivity higher than 95%. In the mixture leaving the isomerization reactor, the molar flowrate ratio $R(\frac{n_{iC_4}}{n_{nC_4}})$, is over 1.5 - 2.0, whereas the iC_4 - molar fraction is around 0.65.

In the one-column process alternative, this unit is responsible for both, the required purity of the iC_4 - product and the low iC_4 - concentration in the feed to the isomerization reactor. Deisobutanizer column is strongly energy-consumer operation so, it has two important consequences for the process economy: i) the cost of having low-content iC_4 - feed to the isomerization reactor is elevated, and ii) the low conversion of the isomerization causes high nC_4 - concentration in the reactor outcome mixture, which is responsible for large recycles and, consequently, large energy consumes for ensuring the iC_4 - product with the desired purity.

The next model was used in Aspen Plus for optimizing the isomerization reactor operation (Figure 7).

Fractional conversion of the reactor was calculated by a user model implemented in VBA by using an equation like (1). The MS Excel application and the simulator were properly connected. An optimization procedure based on the Compass Search algorithm (Davidon, 1991) was also programmed in VBA to carried out the process optimization. The isodebutanizer output stream (COLOUT) was defined according to the information given in Table 1. These data are common in industrial processes of this kind [3,12,16,17,27].

In this case 3, the isomerization reactor was assumed to operate under isothermal conditions for ensuring the temperature was defined univocal- and unambiguously. Thus, two utility services were considered and costed: medium pressure steam for heating the COLOUT stream up to the reactor operating temperature (REACIN) and cooling water for ensuring its isothermal operation.

Due to the lack of confident experimental data, the user model for estimating the fractional conversion as a function of the temperature and the iC_4 - molar fraction (eq. 1), was created with the information generated by an equilibrium calculation using the Equilibrium reactor model in Aspen HYSYS. As usually, the equilibrium conversions in Aspen HYSYS are obtained from the equilibrium constants (K_p) which are computed by equation (3).

$$\Delta G^0 = \sum_i G_i^0 = -R.T \cdot \ln(K_p) \quad (3)$$

where G_i^0 are the standard free energies of the nC_4 - and iC_4 - stored in the HYSYS Databanks.

$$G_i^0$$

The Aspen Plus model shown in Figure 7 was fed with the information on the fractional conversion generated by Aspen HYSYS and reflected in the form described by the eq. (1).

Figures S8 and S8 show that the fractional conversion of nC_4 - to iC_4 - is a lineal function of both the temperature and the molar ratio $R(\frac{n_{iC_4}}{n_{nC_4}})$ at the reactor feed for the intervals evaluated of these variables. These results suggest that fractional conversion of nC_4 - to iC_4 - ($X(nC_4)$) can be predicted by the empirical model given by eq. (4).

$$X_{nC_4} = 0.84550060 - 0.00109878.T - 0.13784487.R(\frac{n_{iC_4}}{n_{nC_4}}) - 0.00118546.T.R(\frac{n_{iC_4}}{n_{nC_4}}) \quad (4)$$

where T is the reaction temperature (in °C) and n_{iC_4} - and n_{nC_4} - are the molar flows of iC_4 - and nC_4 -, respectively, in the isomerization reactor feed.

The adjustable parameters in (4) were obtained by non-linear regression by using the Levenberg-Marquardt algorithm (Marquardt, 1963). A statistical analysis of both the model and the parameters confidence was carried out (Table S2). It showed that not only the parameters but also the whole model result to be statistical meaningful whenever their corresponding p-values are lower than the value of the level of significance (α). In this work, α was set to 0.05.

For the economic analysis of the process shown in Figure 7, four cost elements were considered: i) that one of obtaining an input stream (COLOUT) having a specific iC_4 - molar fraction, ii) the heating cost of the mixture to be fed to the isomerization reactor, iii) the cooling cost at the reactor, to ensure the isothermal operating conditions, and iv)- the cost of a product stream

having a specific n_{C_4} - content. Total operating costs were obtained according to eq. (5).

$$TOC = Cost_{COLOUT} + Cost_{Heating\ Utility} + Cost_{Cooling\ Utility} - Cost_{REACOUT} \quad (5)$$

where all the terms are given in \$/h.

The heating and cooling costs, $Cost_{HeatingUtility}$ and $Cost_{CoolingUtility}$ in eq. (5), respectively, were obtained from the utility cost calculations supported by the Aspen Plus model through automation. High pressure steam and cooling water were selected as heating and cooling media, respectively, having the specifications given by default in the Process Utility Manager in Aspen Plus v 12.1.

The "value" of the input and output streams to the isomerization section (COLOUT and REACOUT, respectively, in Figure 7) depend on the i_{C_4} - and n_{C_4} - mole fractions they, respectively, have. These costs were estimated from the utilities' costs of the deisobutanizer column. In this calculation, a column of certain invariable dimensions was considered (Table S3). Thus, the equipment cost was considered fixed, being the cost of obtaining the desired streams is only dependent on the energy consumes at the condenser and reboiler of the column. The stream fed to the deisobutanizer was described in Table S1, whereas Table S3 shows the column specifications.

$Cost_{COLOUT}$ in eq. (5) increases as lower its i_{C_4} - content is (Figure S10). This dependence can be expressed by eq. (6), where K_1 is an arbitrary parameter.

$$Cost_{COLOUT} = K_1 \cdot 26.39014 \cdot x_{iC_4}^{-0.28834} \quad (6)$$

where x_{iC_4} is the i_{C_4} - molar fraction at the bottoms of the column.

On the other hand, the higher the n_{C_4} - concentration (as result of lower reactor conversion) in the REACOUT stream the lower the value of $Cost_{COLOUT}$ is. This because more energy consumption will be required in the deisobutanizer column to obtain an i_{C_4} - product with the required purity (Table S3). Correspondingly, the value of term $C_{REACOUT}$ in eq. (5) is lower. From the results of the Figure S11, the term $Cost_{REACOUT}$ in eq. (5) can be calculated by the eq. (7).

$$Cost_{REACOUT} = K_2 \cdot (-44.44096 \cdot x_{nC_4}^2 - 0.00099 \cdot x_{nC_4} + 41.06606) \quad (7)$$

where: K_2 is, again, an arbitrary parameter and x_{nC_4} is the n_{C_4} - molar fraction at the reactor outlet stream.

Tailoring conveniently the values of K_1 and K_2 in equations (6) and (7), respectively, the terms $Cost_{COLOUT}$ and $Cost_{REACOUT}$ in eq. (5) are of the same order of magnitude, which is important to ensure their correct contributions to the economic balance of the isomerization unit (Figure 8).

The aim of this case is to minimize the value of TOC of the isomerization unit, calculated by the eq. (5), by varying the i_{C_4} - molar fraction in the mixture fed to the reactor and the operating temperature in the reactor. The next three restrictions were imposed to the optimization: $TOC > 0$, $X(n_{C_4}) > 0.55$ and $R(\frac{n_{iC_4}}{n_{nC_4}}) > 1.5$ in the REACOUT stream (R_{OUT}).

The block diagram used for designing the Excel-VBA application is shown in Figure 3. In this case, Module TIPOS was used for identifying a user-define data type variable. After reading the main input data, the control of the applications was transferred to OPTIN, which controlled the access to CPSEARCH where the Compass Search Procedure was defined Function to

be optimized and its constraints were defined in DFCOMPASS.

A file template which allows building the final application can be used (Figures S12 to S15). Again, a sheet was defined: COMPUTATIONS, where K_1 and K_2 can be introduced. The name and allocation of the Aspen Plus file used in the Automation process should be also introduced before proceeding with the simulation (bkp extension). Specifically:

Module WAYIN, including the following sentences:

File allocation, connection, and application visible

FASP = Cells(3, 2) ' .BKP EXTENSION

Set ihAPsim = GetObject(FASP, "Apwn.Document.39.0")

IhAPsim.Visible = True

Input data

VAR.K1 = Cells(6, 2)

VAR.K2 = Cells(7, 2)

Constant flow rates

VAR.FMOLAR(1) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\C3").Value

VAR.FMOLAR(3) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\IC4=").Value

VAR.FMOLAR(4) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\1C4=").Value

VAR.FMOLAR(5) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\NC4=").Value

VAR.FMOLAR(6) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\TR2C4=").Value

VAR.FMOLAR(7) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\CIS2C4=").Value

VAR.FMOLAR(8) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\NC5=").Value

VAR.FMOLAR(9) = ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\WATER").Value

Call to optimization procedure

Call WAYIN

On-screen computer output

Sheets("COMPUTATIONS").Select

Cells(11, 2) = VAR.IC4

Cells(12, 2) = VAR.T

Cells(15, 2) = VAR.TOC

Cells(16, 2) = VAR.COLOUT

Cells(17, 2) = VAR.CHEATUTIL

Cells(18, 2) = VAR.CCOOLUTIL

Cells(19, 2) = VAR.CREACOUT

Cells(21, 2) = VAR.XIC4COLOUT

Cells(22, 2) = VAR.XIC4REACOUT

Cells(25, 2) = VAR.R

Cells(26, 2) = VAR.ROUT

Cells(27, 2) = VAR.NC4CONV

Cells(28, 2) = VAR.ITERACIONES

Module DFCOMPASS, including the following sentences:

Subroutine where the function (F) to be minimized is written and variables definition.

Public Sub funobj(X() As Double, F As Double)

Dim X1 As Double, X2 As Double, X3 As Double, X4 As Double, X5 As Double, Y1 As Double, Y2 As Double

Dim XNC4 As Double, T As Double, R As Double, XCONV As Double

Dim I As Integer, SUM As Double, XIC4 As Double, XIC4OUT As Double

Dim XNC4OUT As Double

Transfer of data

T = X(2)

If R <= 0 Then R = 0.0000000001

VAR.FMOLAR(2) = X(1)

R = VAR.FMOLAR(2) / VAR.FMOLAR(5)

VAR.IC4 = VAR.FMOLAR(2)

VAR.T = T

VAR.R = R

XIC4OUT = ihAPsim.Tree.FindNode("\Data\Streams\REACTOUT\Output\MOLEFRAC\MIXED\IC4-").Value

XNC4OUT = ihAPsim.Tree.FindNode("\Data\Streams\REACTOUT\Output\MOLEFRAC\MIXED\NC4-").Value

VAR.XIC4REACOUT = XIC4OUT

SUM = 0

For I = 1 To 9

SUM = SUM + VAR.FMOLAR(I)

Next I

XNC4 = VAR.FMOLAR(5) / SUM

XIC4 = VAR.FMOLAR(2) / SUM

VAR.XIC4COLOUT = XIC4

Independent variables

ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\IC4-").Value = VAR.FMOLAR(2)

ihAPsim.Tree.FindNode("\Data\Blocks\REACTOR\Input\TEMP").Value = T

ihAPsim.Tree.FindNode("\Data\Blocks\HEATER\Input\TEMP").Value = T

ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\NC4-").Value = VAR.FMOLAR(5)

Conversion

XCONV = 0.8455006 - 0.00109878 * T - 0.13784487 * R - 0.00118546 * T * R

If XCONV < 0 Then XCONV = 1E-40

ihAPsim.Tree.FindNode("\Data\Blocks\REACTOR\Input\CONV\1").Value = XCONV

VAR.NC4CONV = XCONV

Run

ihAPsim.RUN

Application.Wait (Now + TimeValue("00:00:01"))

Costs

If XIC4 <= 0 Then XIC4 = 1E-20

If XNC4OUT <= 0 Then XNC4OUT = 1E-20

VAR.COLOUT = VAR.K1 * 26.39014 * XIC4 ^ (-0.28834)

VAR.CREACOUT = VAR.K2 * (-44.44096 * XNC4OUT ^ 2 - 0.00099 * XNC4OUT + 41.06606)

VAR.CCOOLUTIL = ihAPsim.Tree.FindNode("\Data\Results Summary\Utility-Sum\Output\TOT_COOL_COST").Value

VAR.CHEATUTIL = ihAPsim.Tree.FindNode("\Data\Results Summary\Utility-Sum\Output\TOT_HEAT_COST").Value

Function to be optimized

F = VAR.COLOUT - VAR.CREACOUT + VAR.CCOOLUTIL + VAR.CHEATUTIL

VAR.TOC = F

In subroutine defined as Public Sub FDESIG(X() As Double, G() As Double), the following constraints are included:

G(1) = -F

G(2) = 0.55 - XCONV

G(3) = 1.5 - VAR.ROUT

G(4) = 145 - T

Finally, Figure 9 show the results obtained from the Aspen Plus interaction after 38 iterations. A minimum was found for TOC = 9.208 \$/h, $X(\text{nc}_4) = 0.593$, $R(\frac{n_{\text{ic4}}}{n_{\text{nc4}}}) = 0.302$ in stream COLOUT (R_{IN}) and $R(\frac{n_{\text{ic4}}}{n_{\text{nc4}}}) = 2.196$ in stream REACOUT (R_{OUT}). The process performance for the minimum operating cost is consistent with the industrial results referred above.

Table 1S: Case 3. Conditions and composition of the mixture (COLOUT in Figure 7) fed to the isomerization reactor. It corresponds to the bottoms of the isodebutanizer column shown in Figure S7.

Variable	Value
Temperature, °C	75.0
Pressure, bar	30
Component molar flows, kmol/h	
iC4-	Variable: 15 to 150
iC4=	6.657
1C4=	7.525
nC4-	177.492
tr2C4=	14.793
cis2C4=	11.436
nC5-	0.398

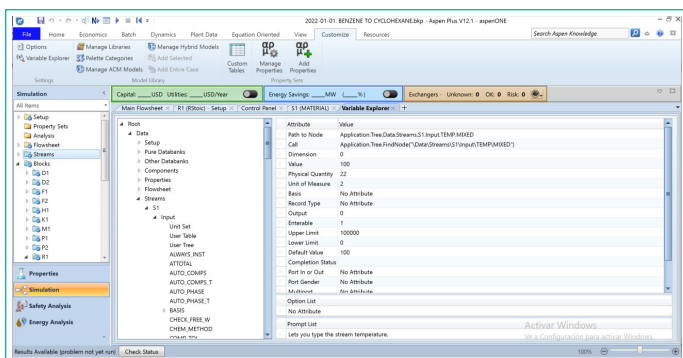


Figure 1: Location of variables for Automation in Aspen Plus.

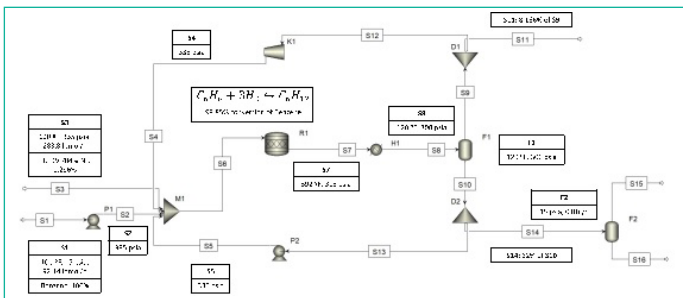


Figure 2: Aspen Plus flowsheet of Case 1: cyclohexane production from benzene. SX: represents stream SX in the flowsheet; P1 is pump P1; M1 is a mixer of streams S2, S3, S4 and S5; R1 is a conversion reactor; H1 is a cooler of the stream S7 exiting from the reactor; F1 and F2 are separators of the Vapour-Liquid streams S8 and S14, respectively; D1 and D2 are stream splitters; K1 is a compressor for the recycle stream S12; P2 is a pump for the recycle stream S13.

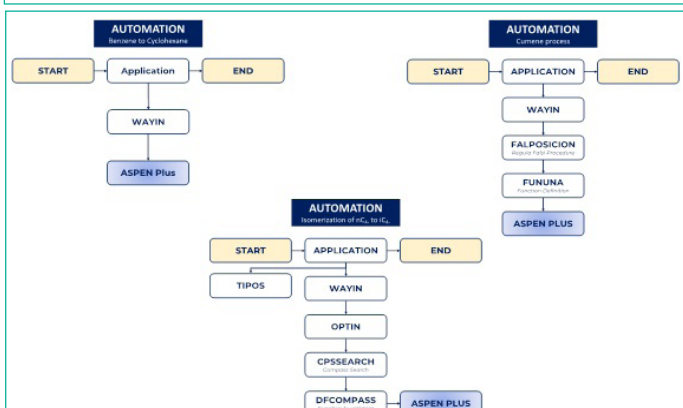


Figure 3: Block diagram corresponding to Cases 1 to 3.

AUTOMATION COMPUTATIONS					
Aspen file:	Mac\Home\LV\UCLM\REVISTED\RESEARCH\UCLM\Education\2021\Automation Aspen\2023-01-01_BENZENE TO CYCLOHEXANE.RKP				
Conversion	Reactor (Btu/h)	yz2 in S11	yCHEX in S16		
0.9975	-4754561.07	0.8914	0.9981		
0.99	-4574320.17	0.9137	0.9873		
0.96	-4377304.26	0.9287	0.9749		
0.94	-4185123.39	0.9383	0.9625		
0.92	-3994911.48	0.9450	0.9489		
0.9	-3805828.68	0.9499	0.9373		
0.88	-3616521.99	0.9537	0.9245		
0.86	-3426978.96	0.9567	0.9116		
0.84	-3236605.94	0.9591	0.8986		
0.82	-3045091.36	0.9611	0.8854		
0.8	-2852137.17	0.9628	0.8721		

Figure 4: Set of input data and results corresponding to Case 1.

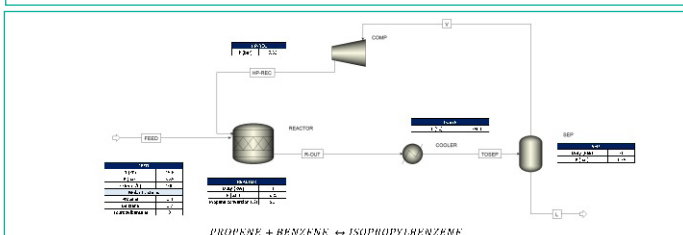


Figure 5: Aspen Plus flowsheet of Case 2: Optimization of the composition of a stream from the production of cumene.

AUTOMATION COMPUTATIONS			
Aspen file: Mac\Home\LV\UCLM\REVISTED\RESEARCH\UCLM\Education\2021\Automation Aspen\2023-02-06_Isopropylbenzene.RKP			
Molar fraction of propene	0.01		
INITIAL ESTIMATIONS			
Tcoolout (°C)	90.0	Molar fraction of propene	0.0199
Tcoolout (°C)	120.0	Molar fraction of propene	0.0077
RESULT			
Tcoolout (°C)	111.8	Molar fraction of propene	0.01000
FUNCTION	5.9501E-07	ITERATIONS	7

Figure 6: Set of input data and results corresponding to Case 2.

OPER		
Name	Units	Value
REACTOR_TEMP	C	145
iC4MolFlowIN	kmol/hr	52.5174
CONV-EQUATION	UNITLESS	0.594461
CONV-REACTOR	UNITLESS	0.594461
iC4FracMolCOLOUT	UNITLESS	0.19404
iC4FracMolREACTOUT	UNITLESS	0.583587
RIN	UNITLESS	0.299112
ROUT	UNITLESS	2.19602

COSTS		
Name	Units	Value
K1	UNITLESS	0.3
K2	UNITLESS	0.5
Cooling	\$/hr	0.19122
Heating	\$/hr	15.2617
UTILITIES	\$/HR	15.4529
ALIM	\$/HR	12.6917
PROD	\$/HR	18.6325
TOTAL	\$/HR	9.51218

Figure 7: Aspen Plus flowsheet of Case 3: Optimization with constraints of the isomerization of nC_4- to iC_4- employing the RSTOIC reactor model. Tables were included for monitoring the results within the Aspen Plus PFD.

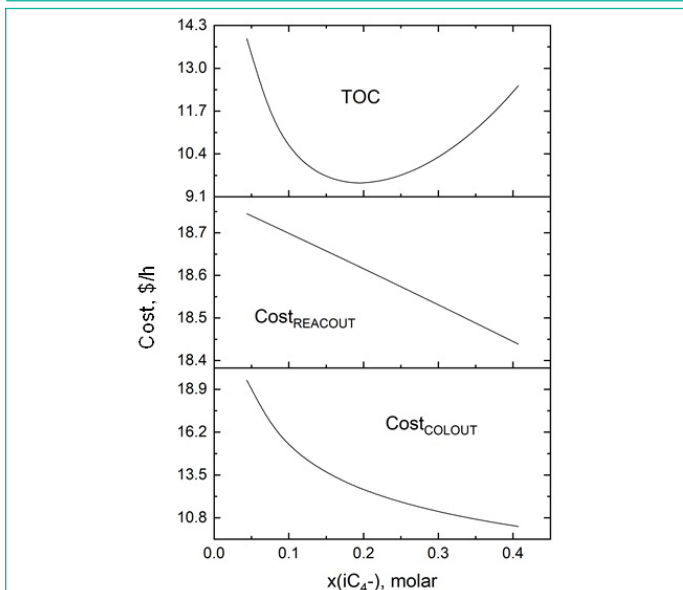


Figure 8: Case 3. Behavior of the terms $Cost_{COLOUT}$, $Cost_{REACTOUT}$ and TOC in the eq. (5) respect to the molar fraction of iC_4- in the feed stream to the isomerization reactor when $K_1 = 0.3$ and $K_2 = 0.5$ in equations (6) and (7), respectively.

AUTOMATION COMPUTATIONS	
Aspen file: C:\BROCA\TOD\BENZENE	
INPUT DATA	
K_1	0.30
K_2	0.50
RESULT	
FUNCTION	1.000000E+00
ITERATIONS	10
CONTROL VARIABLES	
TOC	9.51218
Cost COLOUT	0.19122
Cost Heating Utility	15.2617
Cost Cooling Utility	0.19122
Cost REACTOUT	18.6325
nC_4 COLOUT	0.30
nC_4 REACTOUT	0.583587
RESULT OF OPTIMIZATION	
ROUT (t/h)	2.19602
nC_4 CONVERSION (t/h)	0.19404
ITERATIONS	10

Figure 9: Set of input data and results corresponding to Case 3.

Conclusions

The capability of Automation as a powerful tool for simulating complex processes using Aspen Plus and MS EXCEL-VBA was checked. Three study cases directly taken from literature were considered: the cyclohexane production from benzene and the production of biphenyl (sensitivity analysis), 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-. Detailed information about the correct way to implement Automation by combining the commercial simulator Aspen Plus and MS Excel-VBA was reported.

The experience gained with the development of the examples here reported can be used as the basis for analyzing more realistic cases that commercial software is not able to simulate. Automation can be used for Multi-Disciplinary Analysis Optimization (MDAO), which leads to the communication with external analysis tools and collect the information needed for the optimization design. Other aspect to be considering in future developments is to connect commercial simulators to other third parties like Python or Matlab.

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