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Dynamic Models Towards Operator and Engineer Training: Virtual Environment

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Abstract
The simulation of chemical processes is an important tool for solving problems in Computer Aided Process Engineering (CAPE) and the use of commercial simulators is essential for this task. In this work, the intention is to create a virtual environment for industrial process and data representations for operator and engineer training. The applications focus on the separation process dynamic and control. The first case is an azeotropic distillation process. It was used an industrial plant data to illustrate the importance of reliable thermodynamic data to the process simulation. The system studied is the ethanol/water separation using cyclohexane as mass separating agent. As the second case, it was used a refinery data to simulate the debutanizer column of a fluid catalytic cracking unit in order to make this complex problem understandable, well represented and easily reproducible in a simulation framework. In this case, optimization, regulatory control, PID tuning and model predictive control were considered. The energy consumption was minimized using the SQP method. Simulations were performed using ***HYSYS.Plant*** process simulator.

Keywords: Operator Training, Dynamic Simulation, Control, Distillation Columns

1. Introduction

Operator training and, also, engineer education are areas of interest and importance in industries. These tasks are becoming possible due to the availability of robust software and hardware, and they are extremely important for plant safety, equipment durability and high performance process operation. All of these aspects imply in plant profitability. In this way, virtual plants, using reliable dynamic models, easy interfaces, and vast data bank are important tools.

Dynamic models are used to training exercises, development of process understanding and ability to actuate on critical emergency situations. In this work, two important industrial plants are used to illustrate operator and engineer training benefits. Three steps are highlighted:

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1. rigorous training to assist new operators;
2. physical principles that govern the dynamic behaviour of the process operation;
3. illustration and clarification of control concepts (PID and predictive controllers).

The first application refers to a complete azeotropic distillation process. Industrial plant data were used to illustrate the importance of reliable thermodynamic data to the process simulation. The system studied is the ethanol/water separation using cyclohexane as the mass separating agent. The problem includes different thermodynamic property packages at the same environment (VLE for the distillation columns and LLE for the decanter), azeotrope calculation, equipment and recycling effects.

In the second case, it was simulated a refinery unit, more specifically, the debutanizer column of a fluid catalytic cracking unit (FCCU). In this case, the discussed problems are optimization, regulatory control, PID tuning and model predictive control. The energy consumption was minimized using the SQP method. The process was under product quality restrictions. Steady state simulations were made in order to know the column behavior. The results were analyzed and the top and bottom temperatures were used to maintain the appropriate values of the LPG (liquefied petroleum gas) weathering and the gasoline Reid Vapor Pressure. The reboiler duty and the reflux flow rate were used as manipulated variables. The PID and the model predictive control (MPC) performances were compared. The advantages and disadvantages of each one are discussed.

Simulations were performed using ***HYSYS.Plant*** process simulator. Moreover, both the steady state and dynamic simulation models matched the design data in a high degree of accuracy. In both case studies, the users can note how important is to run plants efficiently and safely.

2. Case Studies

2.1 Ethanol Dehydration

When ethanol is produced by fermentation, the concentration in the outlet of the reactor is about 10% in mass. This mixture is concentrated near to the azeotropic point (89% in mole concentration) in a conventional column and, then from that, it is necessary to use other separation methods to break the azeotrope and to produce pure ethanol. For the azeotropic distillation, cyclohexane is used as entrainer. Table 1 shows the azeotropes in the ethanol/water/cyclohexane system at 1 atm.

Table 1 – Azeotropes in the ethanol/water/cyclohexane system at 1 atm

Azeotropes (mole fraction)	Boiling point (K)	Type
ethanol/water (0.890/0.110)	351.15	Homogeneous
ethanol/cyclohexane (0.449/0.551)	338.15	Homogeneous
water/cyclohexane (0.301/0.699)	343.15	Heterogeneous
ethanol/water/cyclohexane (0.318/0.180/0.502)	335.15	Heterogeneous

Figure 1 shows a schematic flowsheet for the ethanol dehydration. The feed stream composition coming from the fermentation reactor is about 10% ethanol and 90% water (mole basis). Column 1 is a stripper (vapour is fed at the bottom of the column and removes the excess of water). The top product is hydrated ethanol (89% ethanol, mole basis). This stream goes to column 2 (azeotropic column); this column is already fed by a stream containing the entrainer (organic phase recycled from the decanter). The top product composition is near to the ternary azeotrope formed by ethanol, water and the entrainer and the bottom product is pure ethanol. The vapour from the top is condensed and goes to a decanter, where the liquid phase splits into organic and aqueous phases. The organic phase, rich in the entrainer, is recycled to column 1 as reflux and the aqueous phase goes to a recovery column (column 3), where pure water is removed at the bottom and the top product, containing ethanol, water and the entrainer, is recycled back to the azeotropic column.

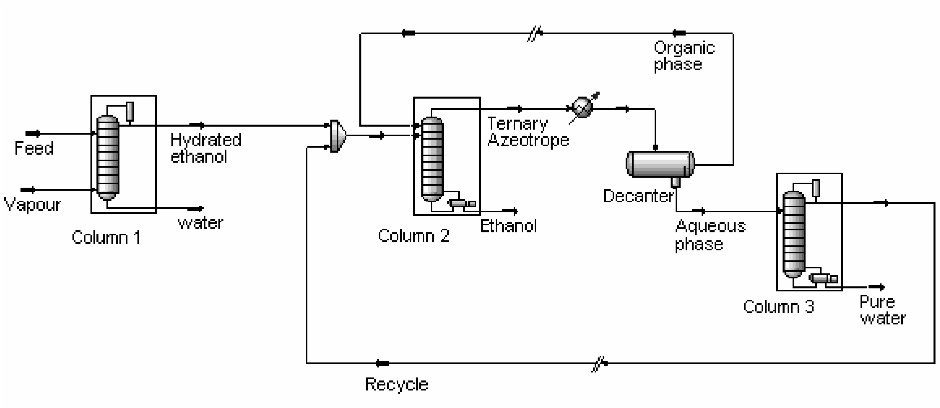

Figure 1 – Ethanol dehydration flowsheet

The start point to obtain a representative model is a reliable database for physical properties and for thermodynamic parameter calculations. In the azeotropic distillation process, this step must be carefully taken into account, because the vapour-liquid equilibrium (VLE), vapour-liquid-liquid equilibrium (VLLE) and liquid-liquid equilibrium (LLE) must be considered. In this way, it must be used different parameters for the decanter and for the distillation columns. Some sets of parameters were tested in order to obtain the ones that could reproduce industrial data (Vasconcelos and Wolf-Maciel, 2002).

Usually, the algorithms used for conventional columns can not support azeotropic distillation. The algorithm used to perform the simu lations was the 'sparse continuation solver' which supports two liquid phases on the trays of the column.

Actual industrial data from a distillery were obtained and the measured values were compared with the simulation results. The design parameters for the process are described in Table 2 and the model validation results are shown in Table 3. An efficiency of 60% (25 theoretical stages) was used to represent the azeotropic column.

Table 2 – Industrial process parameters

Azeotropic column: 42 trays
Recovery column: 21 trays
Bottom pressure: 1.4 atm
Feed flow rate: 8600 Kg/h
Ethanol mass fraction: 93%

Table 3 – Model validation

Temperature (K)	Industrial data	Simulation results
Tray 42	356.45	358.06
Tray 28	346.35	346.15
Tray 9	339.15	339.75

This problem presents interesting aspects reported in Vasconcelos and Wolf-Maciel (2002). One of these aspects is concerned with the multiple steady states. State multiplicity refers to the columns with the same operating conditions and outputs, but with different profiles (Müller and Marquardt, 1997). It is important to introduce an efficient temperature control to assure that the ethanol purity is at the desired value. The main difficulty to control an azeotropic column is due to the strong parametric sensitivity to small variations in the operating conditions (downstream and upstream). With the reliable model presented the operator and the engineer can observe the coupling of variables and the stability conditions. This methodology is being efficiently used in the industry. Besides giving a wide understanding of the whole process, it is being useful to process optimization.

2.2 Debutanizer column

A simplified flow scheme of the debutanizer column is shown in Figure 2. The tower is located in the fluid catalytic cracking unit: naphtha obtained from the reactor cracking is separated into LPG and gasoline. In the overhead section, the non-condensed components are removed as off-gas and this stream is used to control the column pressure. Liquefied Petroleum gas (LPG) is removed as distillate. The column feed is an intermediate stream in the process, so, it is difficult to sample. The alternative is to characterize the products (flowrate and composition) to compose the feed stream.

The objective of the debutanizer column control is to obtain LPG weathering lesser than 2°C and the gasoline RVP lesser than 60 kPa. The debutanizer column control is an important task in petroleum refineries due to the importance of the product quality (Ansari and Tadé, 1998).

Off gas and LPG are analyzed by chromatographic techniques (Table 4). Gasoline and higher hydrocarbons are often characterized using true boiling point curves. The process simulator is able to calculate pseudo-components from the data of Table 5. Table 6 shows the column parameters. The mass flow rates are: Off Gas: 206 ton/day; LPG: 1186 ton/day; Gasoline: 5420 ton/day.

Optimizer

It was used the multi-variable steady state optimizer using the net profit as the objective function. Optimizer uses a spreadsheet for defining the objective function. In this problem, it was used the SQP optimization method and the RVP of gasoline as the constraint. The user must be able to select the method and the associated parameters. The objective function is as follow:

$$\text{Objective function: } \text{Profit} = \sum_{i=1}^{n}(\text{Flowrate} * \text{value}) - \sum(\text{utility costs})$$

Optimization Variables: Reflux ratio and reboiler duty

Results: Top Temperature set point: 334.15K and Bottom Temperature set point: 459.15K

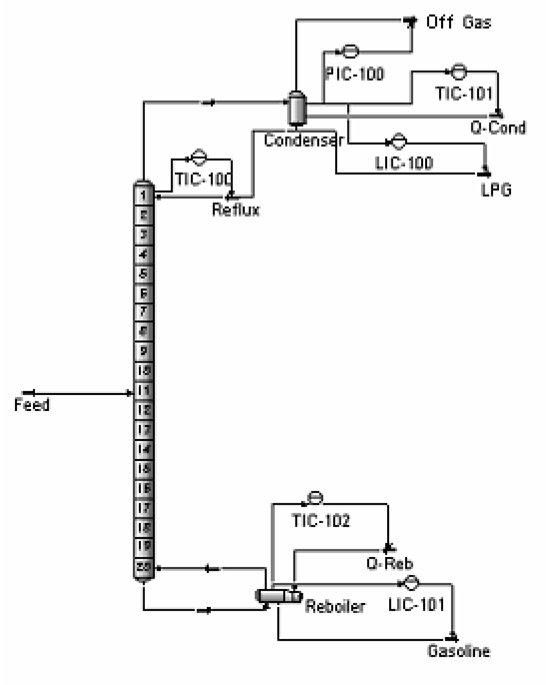

Figure 2 – Debutanizer column control

Table 4 – Offgas and LPG composition

Component	Off-gas % mass	LPG % volume
CO_2	0.01	0.01
H_2S	0.09	0.01
H_2O	0.00	0.05
Etilene	0.07	0.25
Etane	0.11	4.43
Propene	0.35	33.6
Propane	0.14	14.5
i-butane	0.07	14.9
n-butane	0.02	4.63
i-butene	0.14	27.4
1,3-butadiene	0.00	0.11
i-pentane	0.00	0.08

Table 5 – Gasoline true boiling point

% volume	Temperature (K)
0	305.15
5	316.15
10	322.15
20	331.15
30	342.15
40	355.15
50	371.15
60	389.15
70	413.15
80	434.15
90	458.15
95	475.15
100	493.15

Control

Three disturbances were proposed: decrease column feed flow rate (10%), set-point change in the top temperature and increase feed flow rate (22%). The controllers must be able to maintain the controlled variables at the set points and smooth actions in the manipulated variables. The first task is to find the PID tuning parameters to maintain the setpoints. In this problem, it was verified that there was no set of parameters that was able to control the column. It was also used a first order model to the model predictive control. Figures 3 and 4 show the PID and MPC controllers performance for the 22% increase in the feed flow rate. Dashed line represents the bottom temperature and the solid line the manipulated variable (reboiler duty, 10^6 KJ/h).

Table 6 – Column data

Number of stages	20
Feed stage	12
Pressure profile (kg/cm^2_g)	Top = 11.60; Bottom = 11.95
Temperature estimates	Top = 334.15K; Bottom = 458.15K

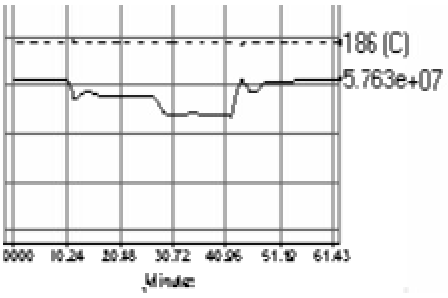

Figure 3 – PID controller performance

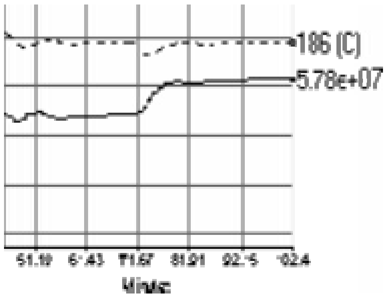

Figure 4 - MPC controller performance

The main features used in this example were: oil characterization (boiling point curve), Optimizer, PID controllers and model predictive controllers.

Also, in this case, the environment was useful not only for operator and engineer training, but also, to optimize the process.

3. Conclusions

The examples illustrated the importance of the simulation facilities for training operators and engineer and also for improving real plant operation. The case studies evaluated are important units in the chemical industries. Furthermore, in the alcohol case, highly non ideal system separation is treated, and in the second case, a not-well defined mixture is studied to process control studies.

4. References

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