

Crude Distillation Process Simulation Using Unisim Design Simulator

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Abstract—The paper deals with the simulation of the crude distillation process using the Unisim Design simulator. The necessity of simulating this process is argued both by considerations related to the design of the crude distillation column, but also by considerations related to the design of advanced control systems. In order to use the Unisim Design simulator to simulate the crude distillation process, the identification of the simulators used in Romania and an analysis of the PRO/II, HYSYS, and Aspen HYSYS simulators were carried out. Analysis of the simulators for the crude distillation process has allowed the authors to elaborate the conclusions of the success of the crude modelling. A first aspect developed by the authors is the implementation of specific problems of petroleum liquid-vapors equilibrium using Unisim Design simulator. The second major element of the article is the development of the methodology and the elaboration of the simulation program for the crude distillation process, using Unisim Design resources. The obtained results validate the proposed methodology and will allow dynamic simulation of the process.

Keywords—Crude oil, distillation, simulation, Unisim Design, simulators.

I. INTRODUCTION

IN chemical and refining industry, the products are produced with precise quality values and at minimal costs. To satisfy these goals, it is necessary to use modeling, simulation, and optimization tools [3].

A chemical simulator is defined as an instrument that solves a complex chemical problem. The core elements of the simulator are [2]:

- Thermodynamic models of the calculation of liquid-vapor equilibrium.
- Components database, which contains the needed values for the calculation of physical properties starting from the thermodynamic models.
- Mathematical model components of the main operating units.
- Flowsheet section that calculates mass balances, energy balances, liquid-vapors equilibrium and composition.
- Output generator section that returns a report of the simulation results.

The modeling and simulation of the crude distillation process may be developed only using simulating software packages. The main worldwide simulators are Aspen Plus, Aspen HYSYS, Unisim Design, and PRO/II.

Aspen HYSYS software has been used to simulate some refinery processes: crude stabilization process, crude oil

stabilization, condensate stabilization, fluid catalytic cracking unit [3]. The research conclusion suggests that modeling and optimization using simulator software can bring new insight in the quest for a better crude distillation process.

Aspen HYSYS Dynamics is another simulation package used to crude oil simulation [6]. The paper describes the best practice for crude fractionation column dynamic modeling, starting from the given crude assay using Aspen HYSYS Dynamics. It includes crude assay characterization, steady state model development, transitioning from steady state model to dynamic model, designing a control strategy for plant disturbances and running the dynamic model.

An example for using of HYSYS v8.6 simulator to Crude Tower is presented in [4]. This reference represents a very good manual to using the HYSYS simulator for crude unit. The most important steps to use in crude oil simulation are:

- Specify components, fluid property packages, and crude oil assays;
- Do characterization calculations, specify crude oil blend, and install into flowsheet;
- Crude Oil Feed and Preheat;
- Atmospheric Distillation Column.

Another simulator for refinery processes simulator is PRO II. This simulator is destined to simulation of chemical processes, but they may be used to refinery processes. An example is represented by the paper of Henry Samueli School of Engineering, University of California [5]. The paper represents an example of crude unit design. The paper describes the next components:

- Process Flow Diagram;
- Pump Calculations;
- Heat Integration;
- Column and Vessel Sizing;
- Priced Equipment List;
- Estimated Plant Cost;
- Product Rates and Properties.

The first four and last components are determined using the numerical results obtained with PRO II simulator.

The good results are obtained with the Petro-SIM simulator [7]. This simulator was selected due to its user friendly Excel™ spreadsheet interface that provides the capability to run multiple cases. The research is focused to optimization of crude distillation process, and the methodology used in the study is defined by the next steps:

- a) develop a set of simulation cases that cover the range of pump around and stripping steam ratios considered;
- b) for each simulation case randomly draw the crude feed composition as well as the crude feed rate;

- c) run process simulations for cases defined above;
- d) use simulation results to build multiple regression models of product yields and crude heater duty requirements as a function of pump around and stripping steam ratios;
- e) generating 3D response surfaces based on the regression models to map out the product yields and the heater duty requirements as a function of pump around and stripping steam ratios;
- f) generating profit response surfaces for market conditions where gasoline margins exceed diesel margins and vice versa;
- g) validating results.

Finally, we have obtained models with multiple linear regression and non-linear regression, including multivariate adaptive regressive splines.

In Romania, the next simulators are used: Petro-SIM used in refineries and Unisim Design in petroleum design companies. In this context, the authors have opted to use in their university the Unisim Design. The author's researches have been oriented to: numerical modeling of vapor-liquid equilibrium by using Edmister - Okamoto model, petroleum fractions liquid – vapor equilibrium simulation using Unisim Design and specific problems of using Unisim Design in the dynamic simulation [8]-[10]. The present paper describes the problems and the results obtained in crude distillation column using Unisim Design simulator.

II. SPECIFIC PROBLEMS OF PETROLEUM LIQUID-VAPORS EQUILIBRIUM

The chemical processes simulation oriented to refinery

processes need the liquid-vapors equilibrium calculus. When is used the Unisim Design simulator, the liquid-vapors equilibrium calculus is conditioned by the configuration steps [9]:

- The chemical compounds selection of the simulator's data base;
- The liquid-vapors equilibrium thermodynamic model selection;
- Chemical compounds concentration setting.

A. Thermodynamic Model Selection

An important problem of the chemical processes simulation is the thermodynamic model selection. For petrochemical and oil and gas applications, the Aspen Hysys Assistant with Property Method Selection recommends the selection of the thermodynamic package Peng-Robinson, especially for hydrocarbons and light gases at medium and low operating pressures [2]. Some properties, as density and transport, are calculated based on American Petroleum Institute procedures.

Another thermodynamic model used in oil and gas application is Chao-Seader model [2]. This liquid-vapors model must be used for heavy hydrocarbons at pressure lower than 0.1 bar and a temperature range of -17.78 to 260 °C (0 to 500 °F). It is strongly recommended for three phase flashes but restricted to the use of pure water in the second liquid phase. It can be used for crude towers, vacuum towers, and ethylene process parts. This model is semi-empirical, based on a wide source of hydrocarbon data.

In this contest, the authors have opted for Peng-Robinson thermodynamic package.

TABLE I
CRUDE OIL PROPERTIES

Fraction	Initial distillation temperature [°C]	Final distillation temperature [°C]	Distillate volume [%]	Cumulated volume [%]	Density fraction
1	30	75	3.6	3.6	0.653
2	75	100	3.3	6.9	0.704
3	100	125	5.0	11.9	0.735
4	125	150	5.7	17.6	0.759
5	150	175	5.8	23.4	0.777
6	175	200	5.6	29.0	0.789
7	200	225	5.7	34.7	0.801
8	225	250	5.6	40.3	0.813
9	250	275	7.7	48.0	0.830
10	275	310	3.0	51.0	0.843
11	310	340	7.0	58.0	0.859
12	347	370	6.3	64.3	0.877
13	370	400	6.3	70.6	0.893
14	400	430	5.2	75.8	0.905
15	-	-	24.2	100.0	0.972

B. Chemical Compounds Characterization

Because of the characteristics of hydrocarbon product, the simulator operates with the pseudo-components in the place of pure chemical components. In these conditions, the simulator configuration is different. The author's researches have evidenced that the switch between the chemical compounds (that exists in data base) with the pseudo-compounds satisfies the next steps [9]:

- The hydrocarbon product properties defining, such as TBP distillation curve, ASTM distillation curve, properties.
- The pseudo-components defining. The pseudo-components are in the boiling point domain of the hydrocarbon product.
- The pseudo-components selection to obtain a distillation curve appropriate to experimental curve.

- The numerical calculus of each pseudo-component concentration by minimizing the difference between the experimental and calculated distillation curve.

The author's experience and Unisim Design simulator manual indications have been synthesized to define the steps necessary to generate the pseudo-components of hydrocarbon products or crude oil [1]:

- The thermodynamic model selection.
- The hydrocarbon lab analysis.
- Load the hydrocarbon product lab analyses in simulator.
- Pseudo-components calculus.
- *Case main* Simulation window definition.
- Liquid-vapors equilibrium calculus.

C. Crude Oil Properties

The author's researches were realized in 2014-2017 period. The start point has been constituted by Romanian crude oil study, characterized by TBP and density curve as shown in Table I [9], [11]. The calculus of the liquid – vapor equilibrium requires following steps:

- a) selecting the thermodynamic model;

- b) load the laboratory analysis in simulator;
- c) selecting the pseudo-components and computing their concentrations;
- d) window *Case main* definition.

D. Pseudo-Components Selection and Concentration Calculus

Determination of the pseudo-components takes place in two stages [9]. In the first stage, the theoretical pseudo-components which correspond to the TBP distillation curve domain are selected. In this example, the oil characterized by the TBP curve described in Table I has been assimilated at a mixture that contain 40 pseudo-components.

The second stage contains the optimal computation of the concentration of each pseudo-component, so that the TBP curve computed based on the pseudo-components is as close as possible to the experimental one. In Fig. 1, the TBP experimental curve is compared with the TBP calculated curve. The graphical image of two distillation curves reflects validation of the pseudo-components selection and concentration calculus.

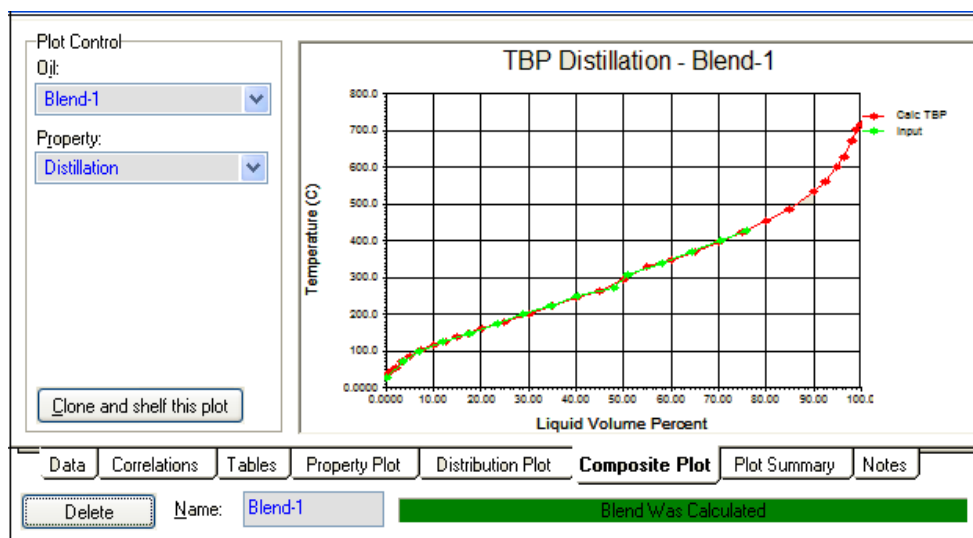


Fig. 1 TBP and experimental curve comparison

III. CRUDE UNIT SIMULATION ANALYSIS

To realize the simulation diagram, the literature reflects some aspects. If Aspen HYSYS simulator is used, it is recommended to use Absorber model [12]. To build the crude distillation unit simulation program using the Aspen HYSYS simulator, the best practice is to build it step by step, making sure that after each step the model is convergent. First, the absorption column model is configured, the feed (crude oil partial vaporized) and the steam used in bottom column are defined. The reflux drum must be configured at tree phasic system as shown in Fig. 2. After the column complete configuration, the model will be simulating to satisfying the convergence criterion.

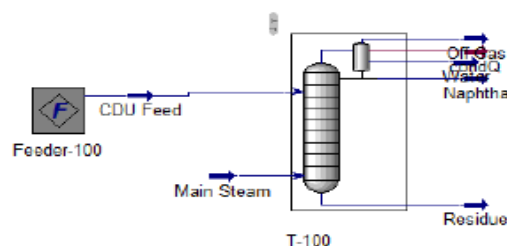


Fig. 2 Initial diagram construction for CDU simulation

If the simulation is finalized with success, the column model is reconfigured by adding the stripper model for kerosene. This new model is then tested. After the model validation, the pumparound is added for the corresponding

kerosene separation column section. The final form of the simulation diagram is presented in Fig. 3.

The HYSYS v8.6 simulator represents another example for CDU detailed simulation [4]. In contrast with anterior

example, the analyzed paper defines the design specifications. The design specifications contain the next elements: Trays & Efficiencies; Condenser Type; Pressures; Temperatures; Feed Locations; Feed Heater; Side Strippers; Pumparound.

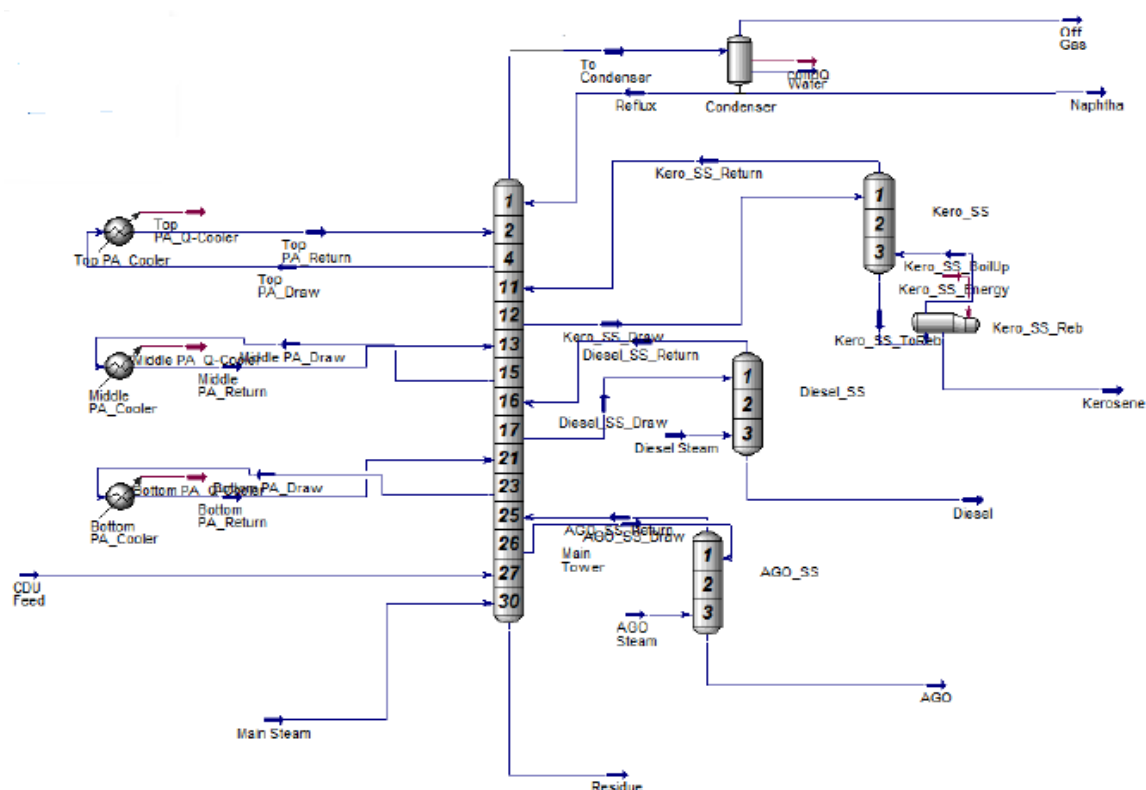


Fig. 3 Final simulation diagram for CDU

In this simulation example, the same model used Refluxed Absorber Column.

A different situation is presented by Aspen Company. The Aspen simulator uses predefined models for crude unit [13]. The simulator manual presents incomplete design specifications and specific configuration commands.

The Honeywell Company proposes a similar programing with Aspen HYSYS [14]. In the analyzed tutorial, the initial model element is the absorption column without reboiler. The design specifications are presented but the configuration commands are detailed. After this analysis, the authors have generated the conclusion of the success of the crude modeling action:

- First component is defined by the design specifications consistency. With a single exception, the author's analysis does not have evidenced an explicit formulation of design specifications of the crude oil distillation column. The authors advance the opinion that the users need the strong examples defined by the design specifications, the developing of the simulation diagram modality and operating scenario simulation.
- Second component used to simulate model configuration is defined by the simulator specific commands used in

configuration operating. This component is better represented in literature [2], but especially by the simulator tutorials [1], [4], [12]-[14].

TABLE II
DESIGN DATA SPECIFICATIONS

Variable	Value
Number of stage	21
Bottoms Liquid Outlet	Heavy distillate
Bottom Stage Inlet	Stripping steam
Optional Inlet Streams/ Stream	Feed
Optional Inlet Streams/ Inlet Stage	17_MAIN TS
Overhead Outlets	Gases
Condenser Energy Stream	Gasoline
Optional Side Draws/ Stream	Qcond
Optional Side Draws/ Type	Kerosene
Optional Side Draws/ Draw Stage	L
Optional Side Draws/ Stream	7_MAIN TS
Optional Side Draws/ Type	Diesel oil
Optional Side Draws/ Draw Stage	L
Optional Side Draws/ Stream	13_MAIN TS

IV. USING UNISIM DESIGN FOR CRUDE DISTILLATION SIMULATION

The author's researches are presented to develop methodology and particular aspects of use Unisim Design to crude distillation simulation.

A. Design Data

The authors have studied a crude distillation column characterized by the design parameters presented in Table II and Table III.

TABLE III
COLUMN PRESSURE GRADIENT

Variable	Value
Condenser Pressure	1.03991
Condenser Pressure Drop	0.39996
Bottom Stage Pressure	1.61053

B. Diagram Simulation Design

The distillation mathematical model is *Refluxed Absorber* object. The model is placed in Unisim Design *Object Palette* menu. The implicit name of the object *Refluxed Absorber* is T-100. In this step, the input and output flows will be configured, using the specified data presented in Table II. Using these elements, the *Refluxed Absorber* configuration

window will have a form presented in Fig. 3. In next step, the bottom pressure will be set, using the value presented Table III.

Because the distillation process is run in steam presence, it is necessary to eliminate. The steam contributes to decreasing the partial pressure and decreasing the boiling point temperature. The introduction in diagram simulation of a three-phase separator is realized in the following steps:

- Open the simulation column window using *Column Environment...* function.
- The actual condenser (biphasic) is deleted and *Object Palette* object is opened and the *3-Phase Condenser* object is selected.
- The condenser menu is opened and the flows that leave the condenser are defined.
- After complete condenser configuration, return to simulation menu of *Column Environment*.

After condenser redefining, the user accesses the *Column Environment* menu, where it will active the *Pressures* option of *Design* menu. This command will define the stages pressures. Because the bottom pressure is already set, there will be only top column pressure. In this mode, the stage pressures are calculated by simulator as shown in Fig. 5.

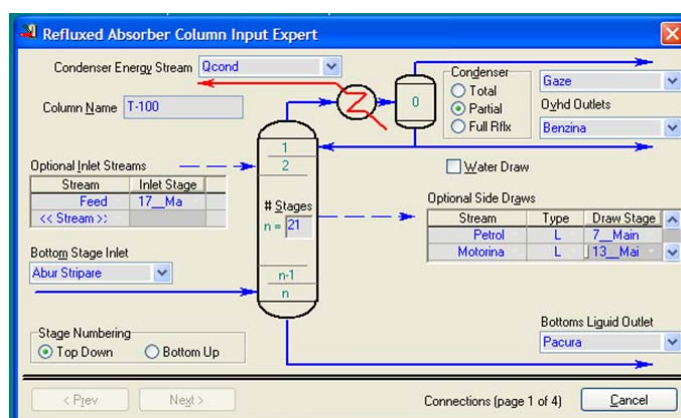


Fig. 4 *Refluxed Absorber* object at end operation of *Connections (1)*

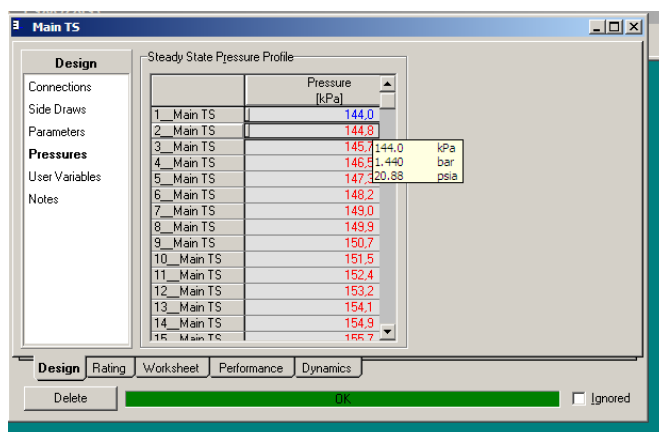


Fig. 5 Colum pressure configuration

V.SIMULATION RESULTS

The distillation column simulation has the scope to study the disturbances and manipulated variables influence of the output process variables. For crude distillation column, the output variables are represented by product qualities. For hydrocarbon products, the quality is represented by ASTM initial and final temperature, density, viscosity and color indices.

The ASTM final product temperatures are calculated by

simulator and they are evidenced using the next procedure:

- Accessing the *Plots* submenu of column *Parent Environment* group using baton *View Table...* of *Assay Curves* window as shown Fig. 6.
- Defining calculus function of the hydrocarbon product properties, respectively *Boiling Point Properties*, using *Profile Data Control...* command as shown Fig. 7. Using the data, the ASTM final product temperature is extracted.

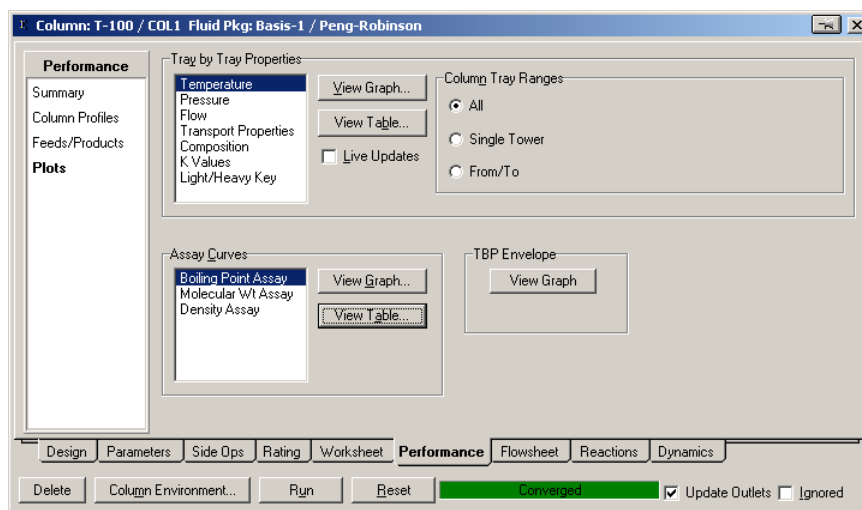


Fig. 6 Selection of Assay Curves function of product

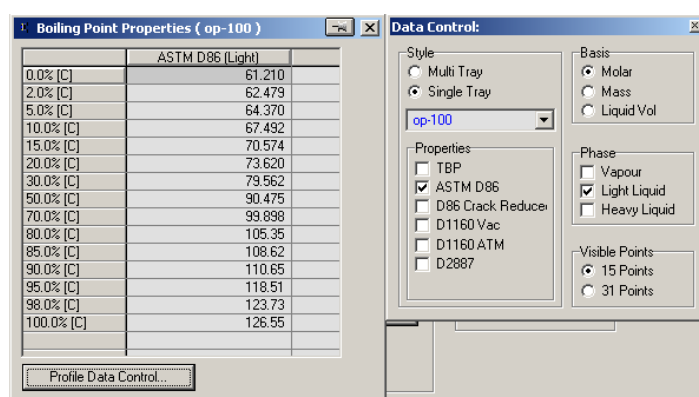


Fig. 7 ASTM gasoline profile temperature

TABLE IV
ASTM FINAL PRODUCT TEMPERATURE

Product	Final temperature [°C]
Gasoline	126.5
Kerosene	236.0
Diesel oil	329.0
Heavy distillate	609.6

Using the function anterior described, the ASTM final product temperatures of all distilled products are collected as listed Table IV. Using this technique, the product flowrate influence to ASTM final temperature of the same product is

determined. Table V presents the numerical results obtained, then product flowrate decreases.

TABLE V
INFLUENCE OF FLOWRATE TO ASTM FINAL PRODUCT TEMPERATURE

Flowrate	Gasoline	Kerosene	Diesel oil
0%	126.5	236.0	329.0
- 5%	126.7	236.6	329.1
- 10%	126.9	237.3	329.2
-15%	127.1	238.0	329.6
- 20%	127.3	238.8	330.1

The crude distillation simulation developed by authors has

one error, because the column simulation program does not product strippers. In future, the strippers will be introduced into diagram simulation.

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