

A MODEL FOR THE DYNAMIC SIMULATION OF A CRUDE OIL UNIT

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Abstract: This paper presents a dynamic model for the crude oil distillation unit. After years of experiments, our model is a compromise between a good results accuracy requiring a complex model and its reasonable dimensions. Because we used DIVA simulator that is “block oriented”, the models representing the main column, sidestrippers, pumparounds and condenser with the tank, describe the plant; the whole unit is represented by these connected elements. At the final of this work we present some simulation results.

Keywords: crude oil unit, nonlinear model, structural approach, dynamic simulation.

1. INTRODUCTION

The crude oil unit, as a part of the Atmospheric and Vacuum Distillation unit, is one of the most important plants in a refinery. Due to its own place (its products being feeds for other important units) and complexity, it is very important to have a powerful instrument to study intimately this multi-component distillation process.

Thus, a software simulator focused on the process dynamics can be one of these analyzing tools; furthermore it can be used not only for research purposes, but also as a support for plant operators training, giving a good way for safe “experiments” of various operating strategies. A special case are the researches for design the control structure of the plant, this way being possible to test its performances before implement it effectively and make improvements if needed.

There is an alternative: to use an “industrial”, “factory made” simulator covering a large class of applications or to build-up a personal one, focused only on the problems regarding the crude oil unit. Obviously, for research purposes, which need a very close “look inside the process”, a dedicated

tool is required, having different features from the general simulators. This way, using an appropriate model, the user is able to know the basics of the distillation process and even to improve the model itself – something impossible in the case of the “industrial” simulators that offer some standard, inflexible models and nothing more.

In order to have the benefits of a dedicated simulator it is necessary to build-up a mathematical model for the process, then to find an appropriate method to integrate it and finally to display the simulation results in an accessible form for the user.

After years of experiments in this field, the authors present in this paper a model for the crude oil distillation unit and suggest a modern solution to integrate it and display/analyze the simulation results. We used a very powerful software oriented on dynamic simulations for industrial plants, DIVA, developed at the Stuttgart University, Germany.

2. THE MATHEMATICAL MODEL FOR THE CRUDE OIL UNIT DYNAMICS

It is quite difficult to build-up a dynamic model for the multi-component distillation due to the process complexity and the problems which may affect the numerical integration of the model equations even using “top level” algorithms and powerful digital equipments.

We propose a model representing a compromise between good results accuracy and a reasonable model dimension in order to require a non-prohibitive execution time for the integration routine. Based on our own experience and literature study too (Chung, Riggs, 1995), we have some simplifying assumptions:

- perfectly mixed component on column trays;
- equilibrium (theoretical) trays;
- negligible vapor holdups;

- constant pressure profile;
- total condenser with “perfect” controlled temperature.

These assumptions lead to a robust model, that can be used in a simulation software environment. It is revealed as an reasonable-dimensional model, but having a good behavior that follows the basic characteristics of the distillation process.

As shown in figure 1, the crude oil unit consists in one main column with two pumparounds and four sidestrippers; the top vapor is totally condensed and stored in a tank where the water is decanted; a part of the top product turns back into the column as external reflux.

The model for the entire unit is obtained from the models for each particular element of the plant as shown as follows.

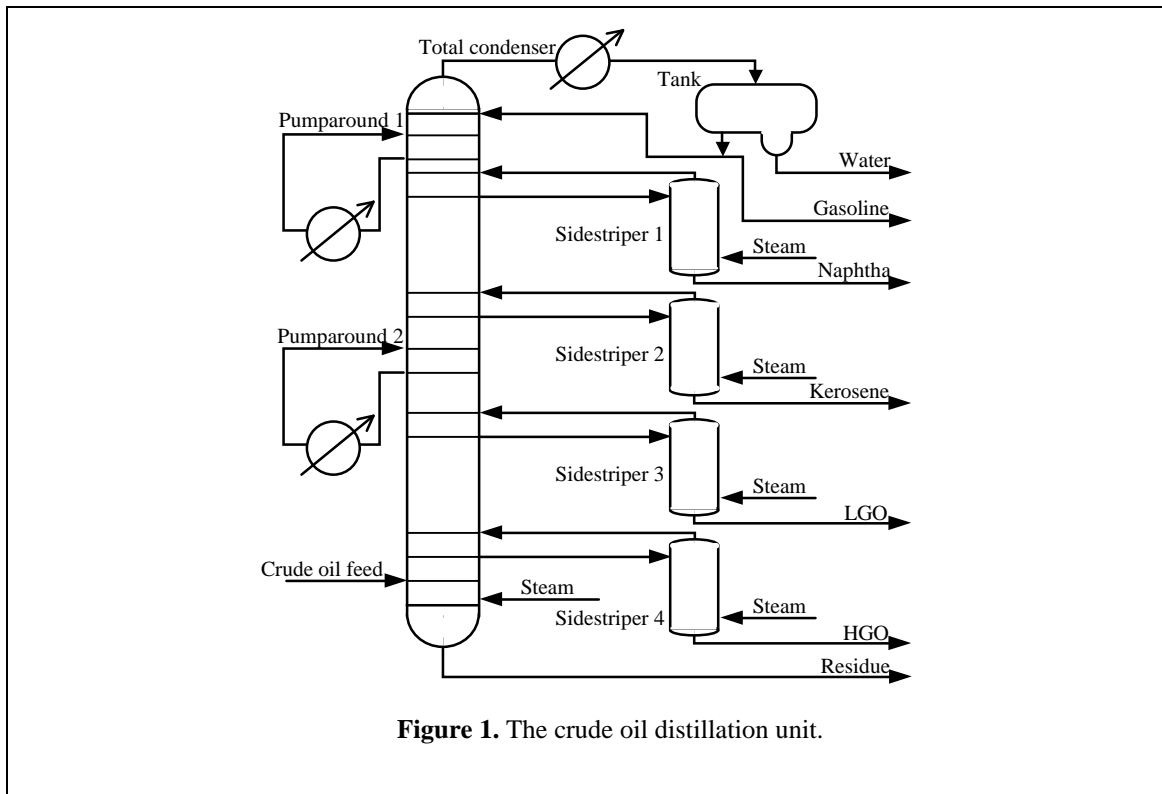


Figure 1. The crude oil distillation unit.

2.1. The columns and sidestrippers

The model for the main column and the sidestrippers is the same, the only thing that differs being the number of trays (considered as a “structural parameter” for the model). It is mainly based on equations for total material balance, component material balance, energy balance and liquid-vapor equilibrium:

? Column top_ (k = 1, see figure 2a):

$$\begin{aligned}
 m_1 \dot{X}_{1,i} &= FL_1 \cdot XFL_{1,i} + FV_1 \cdot YFV_{1,i} + \\
 &+ V_2 \cdot K_{2,i} \cdot X_{2,i} - VE_1 \cdot K_{1,i} \cdot X_{1,i} - \\
 &- X_{1,i} \cdot (FL_1 + FV_1 + V_2 - VE_1) \quad i = \overline{1, NC-1}
 \end{aligned}
 \tag{1}$$

$$0 = 1 - \sum_{i=1}^{NC} X_{1,i}
 \tag{2}$$

$$0 = Y_{1,i} - K_{1,i} \cdot X_{1,i} \quad i = \overline{1, NC} \quad (3)$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{1,i} \quad (4)$$

$$\begin{aligned} \frac{2}{3} bm_1 \cdot LE_1^{(-1/3)} \cdot \dot{LE}_1 = & FL_1 + FV_1 + \\ & + V_2 - VE_1 - LE_1 \end{aligned} \quad (5)$$

$$\begin{aligned} 0 = & FL_1 \cdot HFL_1 + FV_1 \cdot HFV_1 + V_2 \cdot HV_2 - \\ & - VE_1 \cdot HV_1 - HL_1 \cdot (FL_1 + FV_1 + V_2 - \\ & - VE_1) - \sum_{i=1}^{NC} HLP_{1,i} \cdot \dot{X}_{1,i} \end{aligned} \quad (6)$$

$$0 = m_1 - bm_1 \cdot LE_1^{2/3} - m_{0,1} \quad (7)$$

$$0 = LE_1 - L_1 - DL_1 \quad (8)$$

$$0 = VE_1 - V_1 - DV_1 \quad (9)$$

? *Tray k_i* ($k = 2 \dots NS - 1$, see figure 2b):

$$\begin{aligned} m_k \dot{X}_{k,i} = & FL_k \cdot XFL_{k,i} + FV_k \cdot YFV_{k,i} + \\ & + L_{k-1} \cdot X_{k-1,i} + V_{k+1} \cdot K_{k+1,i} \cdot X_{k+1,i} - \\ & - VE_k \cdot K_{k,i} \cdot X_{k,i} - X_{k,i} \cdot (FL_k + FV_k + \\ & L_{k-1} + V_{k+1} - VE_k) \quad i = \overline{1, NC-1} \end{aligned} \quad (10)$$

$$0 = 1 - \sum_{i=1}^{NC} X_{k,i} \quad (11)$$

$$0 = Y_{k,i} - K_{k,i} \cdot X_{k,i} \quad i = \overline{1, NC} \quad (12)$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{k,i} \quad (13)$$

$$\begin{aligned} \frac{2}{3} bm_k \cdot LE_k^{(-1/3)} \cdot \dot{LE}_k = & FL_k + FV_k + \\ & + L_{k-1} + V_{k+1} - VE_k - LE_k \end{aligned} \quad (14)$$

$$\begin{aligned} 0 = & FL_k \cdot HFL_k + FV_k \cdot HFV_k + \\ & + L_{k-1} \cdot HL_{k-1} + V_{k+1} \cdot HV_{k+1} - \\ & - VE_k \cdot HV_k - HL_k \cdot (FL_k + FV_k + \\ & + L_{k-1} + V_{k+1} - VE_k) - \sum_{i=1}^{NC} HLP_{k,i} \cdot \dot{X}_{k,i} \end{aligned} \quad (15)$$

$$0 = m_k - bm_k \cdot LE_k^{2/3} - m_{0,k} \quad (16)$$

$$0 = LE_k - L_k - DL_k \quad (17)$$

$$0 = VE_k - V_k - DV_k \quad (18)$$

? *Column bottom_i* ($k = NS$, see figure 2c):

$$\begin{aligned} m_{NS} \dot{X}_{NS,i} = & FL_{NS} \cdot XFL_{NS,i} + \\ & FV_{NS} \cdot YFV_{NS,i} + L_{NS-1} \cdot X_{NS-1,i} - \\ & VE_{NS} \cdot K_{NS,i} \cdot X_{NS,i} - X_{NS,i} \cdot (FL_{NS} + \\ & + FV_{NS} + L_{NS-1} - VE_{NS}) \quad i = \overline{1, NC-1} \end{aligned} \quad (19)$$

$$0 = 1 - \sum_{i=1}^{NC} X_{NS,i} \quad (20)$$

$$0 = Y_{NS,i} - K_{NS,i} \cdot X_{NS,i} \quad i = \overline{1, NC} \quad (21)$$

$$0 = 1 - \sum_{i=1}^{NC} Y_{NS,i} \quad (22)$$

$$\begin{aligned} \dot{m}_{NS} = & FL_{NS} + FV_{NS} + L_{NS-1} - \\ & - VE_{NS} - LE_{NS} \end{aligned} \quad (23)$$

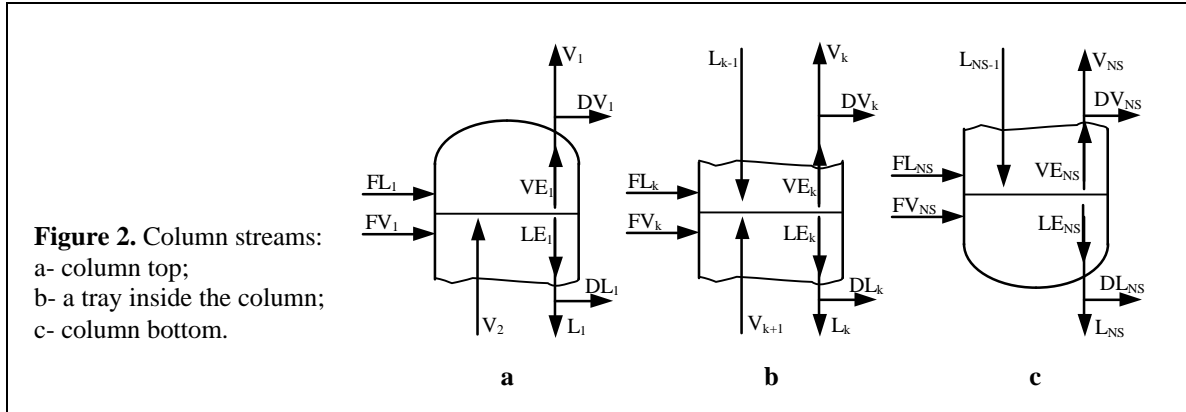
$$\begin{aligned} 0 = & FL_{NS} \cdot HFL_{NS} + FV_{NS} \cdot HFV_{NS} + \\ & + L_{NS-1} \cdot HL_{NS-1} - VE_{NS} \cdot HV_{NS} - \\ & - HL_{NS} \cdot (FL_{NS} + FV_{NS} + L_{NS-1} - \\ & - VE_{NS}) - \sum_{i=1}^{NC} HLP_{NS,i} \cdot \dot{X}_{NS,i} \end{aligned} \quad (24)$$

$$0 = LE_{NS} - DL_{NS} \quad (25)$$

$$0 = LE_{NS} - L_{NS} - DL_{NS} \quad (26)$$

$$0 = VE_{NS} - V_{NS} - DV_{NS} \quad (27)$$

In these equations, the enthalpies and liquid-vapor equilibrium constant must be specified, for example by polynomial functions of temperature (the most simple case) or using some more complex and accurate correlations of pressure, temperature and composition, if enough information is available to the user like Chao-Seader, Boston-Britt a.s.o. (Parekh, 1998; Stratula, 1976; Stratula, 1986).



We must emphasize a few characteristics of this model:

- the system is non-linear, ill conditioned, stiff, due to the different time scales in the model, imposing serious limitations for the integration step in order to have a stable numerical solution;
- a real problem for integration is to find a true steady state, with practical relevance, to use it as a good starting point for the dynamic simulation;
- the transient time has a value in the range of 5...25 hours (for industrial crude oil distillation units);
- the system dimension is very large and may lead to some memory management problems; thus we must operate some dimensional reductions (i.e. observing that only a few trays in the column have external feeds or sidedraws).

2.2. The pumparounds

The model for the pumparounds (figure 3) is mainly based on the equation for the heat transfer from the cooled product stream to the cooling agent, obviously without any changes in product composition and flow rate:

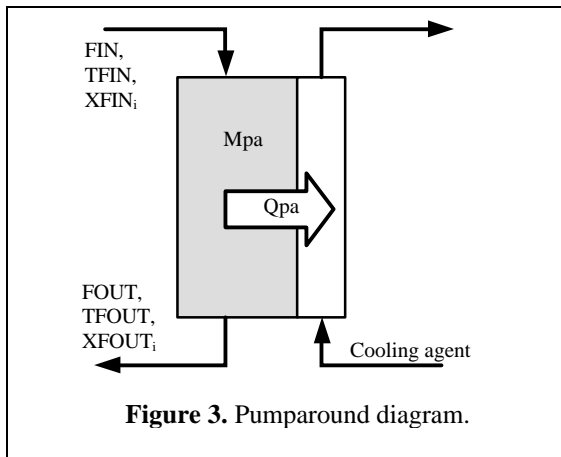


Figure 3. Pumparound diagram.

$$\frac{M_{pa}}{FIN} \cdot \dot{T}_{OUT} = T_{IN} - T_{OUT} - \frac{Q_{pa}}{FIN \cdot c_p} \quad (28)$$

$$0 = X_{IN} - X_{OUT} \quad (29)$$

$$0 = F_{IN} - F_{OUT} \quad (30)$$

2.3. The condenser with tank

For this assembly (figure 4) we adopted a very simple model, considering the case of a total condenser with "perfect" temperature control and constant liquid holdup in the tank (the decanted water accumulation is modeled too):

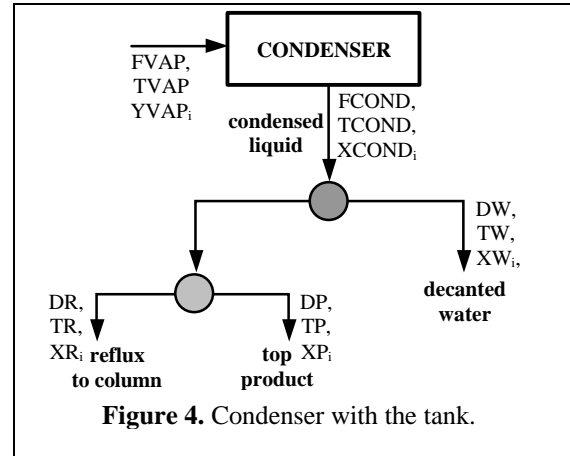


Figure 4. Condenser with the tank.

$$0 = X_{COND_i} - Y_{VAP_i} \quad i = \overline{1, NC} \quad (31)$$

$$0 = T_{COND} - T_{FIX} \quad (32)$$

$$0 = F_{COND} - F_{VAP} \quad (33)$$

$$0 = DW - f_w \cdot F_{COND} \cdot X_{COND_{NC}} \quad (34)$$

$$0 = DP - \frac{F_{COND} - DW}{1 + RR} \quad (35)$$

$$0 = DR - RR \cdot DP \quad (36)$$

$$0 = XR_i - \frac{XCOND_i \cdot FCOND}{FCOND - DW} \quad i = \overline{1, NC - 1} \quad (37)$$

$$0 = XR_{NC} - \frac{XCOND_i \cdot FCOND - DW}{FCOND - DW} \quad (38)$$

$$0 = TR - TCOND \quad (39)$$

$$0 = XP_i - XR_i \quad i = \overline{1, NC} \quad (40)$$

$$0 = TP - TCOND \quad (41)$$

$$0 = XW_i \quad i = \overline{1, NC - 1} \quad (42)$$

$$0 = XW_{NC} - 1 \quad (43)$$

$$0 = TW - TCOND \quad (44)$$

The Chung-Riggs model is the basic model in the literature, of course, with a few variations. It is well accepted considering its performances and reasonable dimensions. Our model is in fact based on their model; the most significant changes are the new form of the equation (24) – in our model it is an algebraic equation, not a differential one like in Chung-Riggs model – and a new model for the total condenser with the tank. These changes reduce the computational effort and improve the behavior of the model.

Obviously the model had to be validated, in order to be sure it is accurate to provide solutions with practical relevance. In the same time we had to evaluate how far we can go with our simplifying assumptions.

The authors were in the situation to find an appropriate way to validate the mathematical model. In a “normal” situation, having reasonable dimensions and complexity, there are available a few analytical methods to study the inherent model properties: its solutions existence, uniqueness, continuity depending on the input data and especially their behavior in concordance with the physical sense. But unfortunately it is not our case: the model is quite large and complex even for a regular computer-coded representation, not only for a human researcher! This way, the only method to validate the model is to study very carefully its behavior during a significant number of simulations; our opinion is that the model above have a good accuracy as time as there is an obvious concordance between the obtained results and the data directly taken from the real plant, taking into account of the good sense remarks from the plant operators too.

3. DYNAMIC SIMULATION OF THE ENTIRE DISTILLATION UNIT

To simulate the dynamics of the crude oil unit means in fact to integrate its mathematical model equations, requiring adequate routines for numerical integration and graphical representation of the simulation results. The authors of this paper suggest a very versatile and powerful software oriented on dynamic simulations for industrial plants, DIVA (Dynamische Simulation Verfahrenstechnischer Anlagen), developed at the Stuttgart University (Kienle 1997, Köhler 1999, Kröner 1999). This simulator is running under Linux operating system and integrates some sets of high-level routines for solve/integrate complex algebraic and differential equation systems. It is not the place here to describe the features of DIVA simulator, but we want to emphasize that, being oriented on simulations over the industrial plants, it works with the concept of “block device”: the entire plant is divided in relevant parts in accord with topologic and functional rules. Every block is described by its own model and external connections, giving a natural way to aggregate the entire plant, a way we call “a structural approach”.

As an example, we present in figure 5 a diagram representing the existing connections between “device-blocks” for the crude oil unit, as it must be specified for DIVA simulator. The blocks are described by the models presented (equations (1)...(44)).

Some remarks have to be done:

- the inputs and outputs for these blocks can be “material” streams (“complex” streams) and “informational” streams (“simple” streams);
- a material stream (thick arrow in the diagram) can be sub-divided in informational streams (thin arrows). This way, all connections between blocks become informational links, but we prefer to use material links too, because our “structural approach” is focused on the easy-to-understand description form for the plant inside the simulator;
- once all needed connections between blocks are established, changing the model for one particular block doesn’t imply any changes in the plant description inside the simulator.

There are some important advantages using this manner of work:

- A very easy to understand representation of the plant;
- An easier way to describe the plant through a mathematical model, using multiple simple models for the blocks instead of a single complex model for the entire plant;

- The user is able to test the parts of the plant and to identify mismatches in the models;

- A possibility to have an open structure that will permit anytime improvements and additional modules.

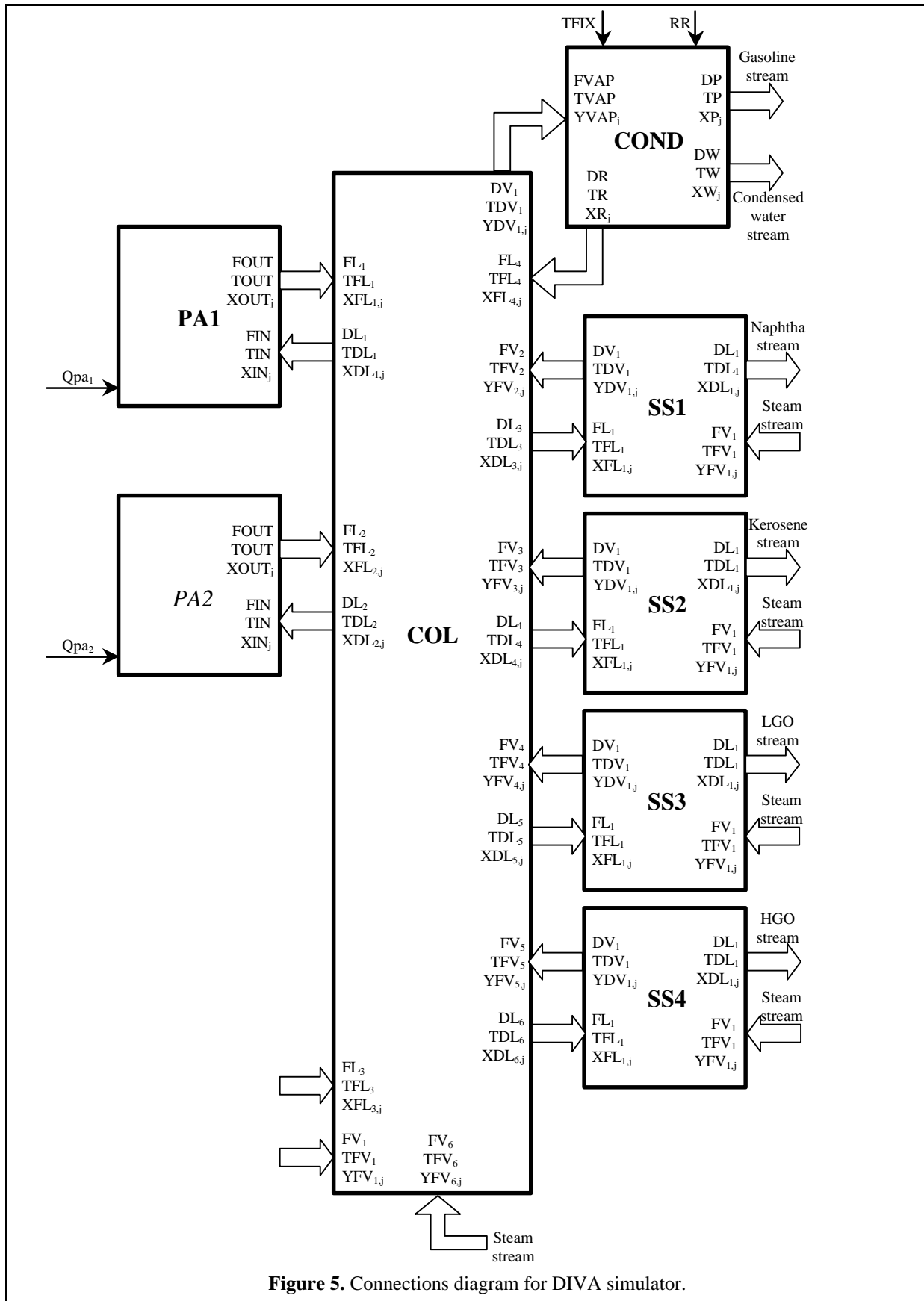


Figure 5. Connections diagram for DIVA simulator.

For detailed information about DIVA simulation environment that include the graphical representation feature (using a dedicated MATLAB toolbox) the reader may consult the references (Kienle 1997, Köhler 1999, Kröner 1999).

We tested our model on an industrial crude oil unit (its structure being shown in figure 1); some significant data are presented in table 1.

Table 1. Some data about the crude oil unit.

Number of trays in the main column	30
Number of trays in the sidestriper	3
Number of pseudo-components in the feed	37, including water
Feed type	pre-flashed
Feed flow rate	0.57 kmol/s
Reflux ratio	0.23
Molar holdup on column trays	3.0 kmol

As example, some diagrams are presented. These simulation results were obtained using our model for the column mentioned above.

Regarding the simulator settings, we used in DIVA the NLEQ1S solver (Newton method with variable damping strategy) to get the initial conditions and LIMEXS integrator (extrapolation method with variable step size).

In figures 6 and 7 is presented the evolution of the component 5 (a light pseudo-component) fraction in gasoline and naphtha after a step increasing in the steam flow rate at the bottom of the column. Due to the stripping effect of the steam, the lighter components are moved to the top of the column, their fraction increases in the top product – gasoline and decreases in the bottom product of the sidestriper 1 – naphtha. The initial “peak” in figure 5 is an effect of the assumption that we have negligible vapor holdups on trays, meaning “instant” vapor propagation from bottom to top.

Figures 8 and 9 presents the temperature evolution in the column top and bottom when external reflux ratio increases. In figure 8 the effect of internal

column interactions can be observed: in the first time interval the temperature decreases (as a direct effect of an incoming colder stream), then it increases and decreases again to a new steady value due to the changes in the column internal flow rates. On tray 30 (column bottom) there is an initial temperature increase (due to the incoming internal stream from above, with higher temperature), but after that the temperature decreases, as an effect of internal liquid stream cooling due to the reflux ratio increase.

These simulation results are significant, at this point, not for analyzing the column dynamic behaviour, but to show how the model implementation in DIVA works. A few experiments proved that the execution time is about 20 times compressed (an hour of column-time is simulated in 3 minutes), even if the whole model consists in about 5000 equations! Another fact to be mentioned is that the simulator implemented in DIVA is only at its “first age” – and there will be a lot of changes in it, improving the performances., but it is very important to show this is a good way to follow.

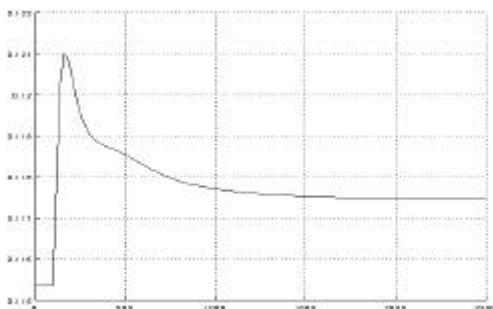


Figure 6. Comp. 5 in top product (gasoline) when steam flow rate increases.

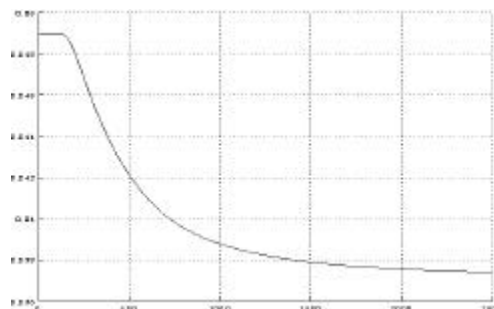


Figure 7. Comp. 5 in bottom of sidestriper 1 (naphtha) when steam flow rate increases.

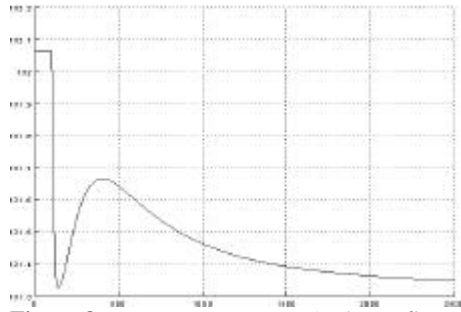


Figure 8. Temperature on tray 1 when reflux ratio increases.

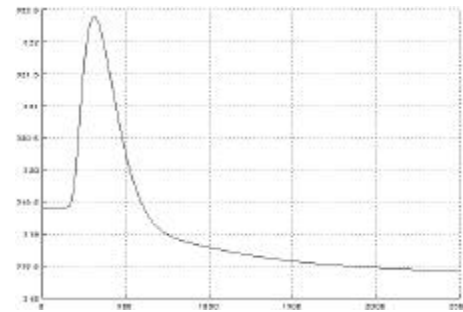


Figure 9. Temperature on tray 30 when reflux ratio increases.

4. CONCLUSIONS

In this paper was presented a dynamic model for the crude oil distillation unit, based on the Chung-Riggs model. The most important change is that the model for the whole plant consists in the models for a few blocks representing elements of the plant: the main column, sidestrippers, pumparounds and condenser with the tank. This partition of the unit in sub-components is very useful for an easy model implementation and integration in DIVA, the software environment we used to simulate the crude oil plant. At the final of our work some simulation results are presented. It shows how our simulator works, even if it is only at the beginning and has to be improved. Our manner of work reveals the advantages of the “structural approach”, which permit a flexible implementation and leads to a very fast simulation.

5. ACKNOWLEDGEMENTS

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NOMENCLATURE

Molar flow rates:

FL – liquid feed on tray;
FV – vapor feed on tray;
LE – liquid leaving the tray;
VE – vapor leaving the tray;
DL – liquid sidedraw from tray;
DV – vapor sidedraw from tray;
L – liquid remaining after sidedraw;
V – vapor remaining after sidedraw;
FIN – product to heat exchanger;
FOUT – product from heat exchanger;
FVAP – vapor to condenser;
FCOND – condensed liquid;
DW – decanted water;
DP – top product;
DR – reflux to the column.

Molar fractions:

XFL – pseudo-component in liquid feed;
YFV – pseudo-component in vapor feed;
X – pseudo-component in liquid on tray;
Y – pseudo-component in vapor on tray;
XIN – pseudo-component in product to heat exchanger;
XOUT – pseudo-component in product from heat exchanger;
YVAP – pseudo-component in vapor to condenser;
XCOND – pseudo-component in condensed liquid;
XR – pseudo-component in reflux to column;
XP – pseudo-component in top product;
XW – pseudo-component in decanted water.

Temperatures:

TIN – product to heat exchanger;
TOUT – product from heat exchanger;
TFIX – setpoint for condensed liquid;
TCOND – condensed liquid;
TW – decanted water;
TP – top product;
TR – reflux to the column.

Molar enthalpies:

HFL – liquid feed;
HFV – vapor feed;
HL – liquid on tray;
HV – vapor on tray;
HLP – pseudo-component in liquid phase.

Others:

K – liquid-vapor constant;
m₀ – constant liquid holdup on tray;
m – liquid holdup on tray;
bm – coefficient in the holdup equation;
NS – number of column trays;
Mpa – product holdup in the heat exchanger;
Qpa – heat exchange on pumparound;
cp – product specific heat;
fw – the fraction of decanted water from condensed liquid.

Indexes:

i – pseudo-component;
k – tray number.

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