An Original Approach for the Dynamic Simulation of a Crude Oil Distillation Plant

I. Building-up a full-scale mathematical model

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A crude oil plant consists of a main column with several sidestripers and pumparounds. While steady state modeling and simulation is fairly standard today, using well-known software tools as HYSYS platform (ASPEN) and PRO/II environment (Simulation Sciences Inc.), only little is known about the dynamic simulation of crude oil plants intimacy in the open literature. Due to the process complexity, the references in this field mention many difficulties in building-up a dynamic model for this multi-component distillation (as first step in the dynamic simulator implementation), model that could be appropriate for numerical integration [1,2]. The presented model is based on pseudo-components and makes use of the well-known MESH equations, in an original approach following topological and functional rules. Additional simplifications result in a robust dynamic model with reasonable accuracy, without affecting the "full-scale" model feature. This first part of the work presents the detailed mathematical model, explicitly oriented to numerical integration within an appropriate simulation environment.

Keywords: crude oil plant, nonlinear models, process dynamics

The crude oil unit, as part of the Atmospheric and Vacuum Distillation plant, is the first processing unit in a refinery. Due to its position (with products becoming either final products or feedstock for other processing units), its complexity and high energy consumption involved, it is very important having powerful instruments to intimately study it.

A dedicated software simulator, focused on the dynamic behavior of this multi-component distillation process, can be one of these analyzing tools. It can be used not only for research purposes, but also as plant operators training support, giving a good way for safe "experiments" of various operating strategies. A special case is represented by the plant control structure design, being possible to test its performances before effectively implement it and make improvements if needed [3 - 6]. Obviously, for a very close "look inside the process" a dedicated tool is required, with different features from the general "large scale applications" simulators. This way, using an appropriate mathematical model, the user is able to know the basics of the distillation process and even to improve the model itself – a non-existing feature in the case of general simulators (offering some standard, inflexible models and nothing more).

In order to build-up a simulator, first it is necessary to aggregate a mathematical model for the process, then to find an appropriate method to solve it and, finally, to display the simulation results in an accessible form for the user. After years of experiments, the author presents in this first part a full-scale model for the crude oil distillation unit (with no dimensional reductions), in a new functional/ topological approach.

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 problems affecting the numerical integration of the model equations, even by using "top level" algorithms and powerful digital equipments.

The author proposes 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. Still the proposed model remains a "full-scale" one, because no dimensional reduction techniques are applied – all model good performances and robustness coming from a judicious equations formulation. Based on own experience and literature study too [1, 2, 7 - 9], some simplifying assumptions have to be made:

-The mixture is "approximated" using the pseudo-components technique [1, 9].

-Perfectly mixed component on column trays.

-Equilibrium (theoretical) trays, with negligible vapor holdups.

-Constant pressure profile.

-Total condenser with "perfect" controlled temperature.

These assumptions lead to a robust and reasonably dimensioned model, but having a good behavior following the basic characteristics of the distillation process.

As shown in figure 1, the crude oil plant considered in this work consists in one main column with two pumparounds and four sidedraws to the sidestripers; 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 [10].

The crude feed was divided into $NC = 37$ pseudo-components (including added water), in order to represent the true-boiling-point (TBP) curve [1, 2, 9, 11], a manner of work extended to all material streams in the plant. The model for the entire unit is obtained from the models for each particular element of the plant as shown there in after.

The columns and sidestripers

The model for the main column and the sidestripers is qualitatively the same; only the number of trays is different and may be considered as a "structural parameter". Equations for total material balance, component material

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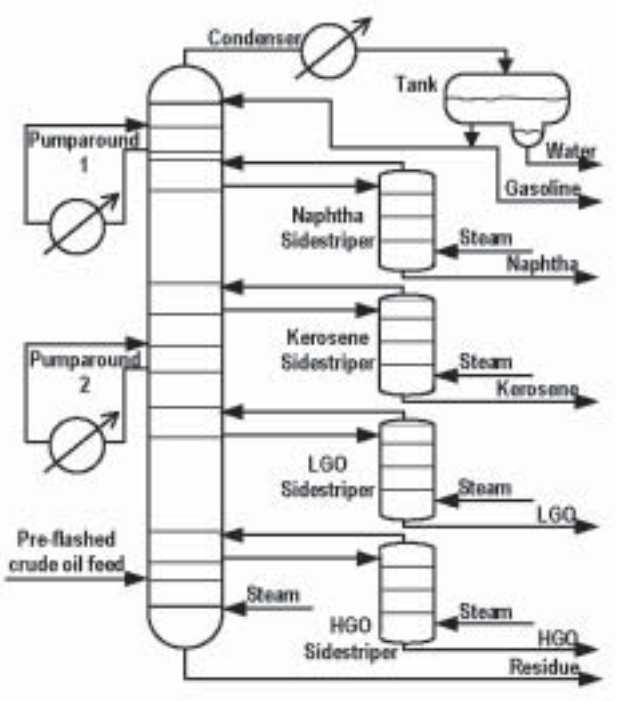

Fig. 1. The crude oil distillation plant

balance, energy balance and liquid-vapor equilibrium are here involved [11-15].

Column top (k = 1, fig. 2a):

Component material balance, with dm_1/dt substituted from the total material balance equation:

$$m_1\frac{dX_{1,i}}{dt} = FL_1\cdot XFL_{1,i} + FV_1\cdot YFV_{1,i} + V_2\cdot K_{2,i}\cdot X_{2,i} - VE_1\cdot K_{1,i}\cdot X_{1,i} - \\ - X_{1,i}\cdot(FL_1 + FV_1 + V_2 - VE_1) \quad i = 1,...,NC-1 \tag{1}$$

Summation condition: $0 = 1 - \sum_{i=1}^{NC} X_{1,i}$ (2)

Phase equilibrium:

$$0 = Y_{1,i} - K_{1,i}\cdot X_{1,i} \quad i = 1,...,NC \tag{3}$$

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

Total material balance, where the left-hand side, dm_1/dt , is substituted from the holdup equation, taking into account in the Francis relation [2, 12, 13, 16]:

$$\frac{2}{3}bm_1\cdot LE_1^{(-1/3)}\cdot\frac{dLE_1}{dt} = FL_1 + FV_1 + V_2 - VE_1 - LE_1 \tag{5}$$

Energy balance, assuming quasi-static temperature changes changes $\left(\frac{dT_1}{dt}\cong 0\right)$ leading to an easier way to solve dynamic model formulation [17]:

$$0 = FL_1\cdot HFL_1 + FV_1\cdot HFV_1 + V_2\cdot HV_2 - VE_1\cdot HV_1 - HL_1\cdot \\ (6)(FL_1 + FV_1 + V_2 - VE_1) - m_1\sum_{i=1}^{NC} HLP_{1,i}\cdot\frac{dX_{1,i}}{dt} \tag{6}$$

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

Liquid and vapor sidedraws:

$$0 = LE_1 - L_1 - DL_1 \tag{8}$$

$$0 = VE_1 - V_1 - DV_1\ . \tag{9}$$

.

The model equations for the inner trays and column bottom are formulated in a similar way:

Tray k (k = 2…NS – 1, fig. 2b):

Component material balance:

$$m_k\frac{dX_{k,i}}{dt} = FL_k\cdot XFL_{k,i} + FV_k\cdot YFV_{k,i} + L_{k-1}\cdot X_{k-1,i} + V_{k+1}\cdot K_{k+1,i}\cdot X_{k+1,i} - \\ - VE_k\cdot K_{k,i}\cdot X_{k,i} - X_{k,i}\cdot(FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k) \quad i = 1,...,NC-1 \tag{10}$$

Summation condition:

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

Phase equilibrium:

$$0 = Y_{k,i} - K_{k,i}\cdot X_{k,i} \quad i = 1,...,NC \tag{12}$$

Summation condition:

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

Total material balance:

$$\frac{2}{3}bm_k\cdot LE_k^{(-1/3)}\cdot\frac{dLE_k}{dt} = FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k - LE_k \tag{14}$$

Energy balance:

$$0 = FL_k\cdot HFL_k + FV_k\cdot HFV_k + L_{k-1}\cdot HL_{k-1} + V_{k+1}\cdot HV_{k+1} - VE_k\cdot HV_k - \\ - HL_k\cdot(FL_k + FV_k + L_{k-1} + V_{k+1} - VE_k) - m_k\sum_{i=1}^{NC} HLP_{k,i}\cdot\frac{dX_{k,i}}{dt} \tag{15}$$

Holdup:

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

Liquid and vapor sidedraws:

$$0 = LE_k - L_k - DL_k \tag{17}$$

$$0 = VE_k - V_k - DV_k\ . \tag{18}$$

.

Column bottom (k = NS , fig. 2c):

Component material balance:

$$m_{NS}\frac{dX_{NS,i}}{dt} = FL_{NS}\cdot XFL_{NS,i} + FV_{NS}\cdot YFV_{NS,i} + \\ + L_{NS-1}\cdot X_{NS-1,i} - VE_{NS}\cdot K_{NS,i}\cdot X_{NS,i} - \\ - X_{NS,i}\cdot(FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS}) \quad i = 1,...,NC-1 \tag{19}$$

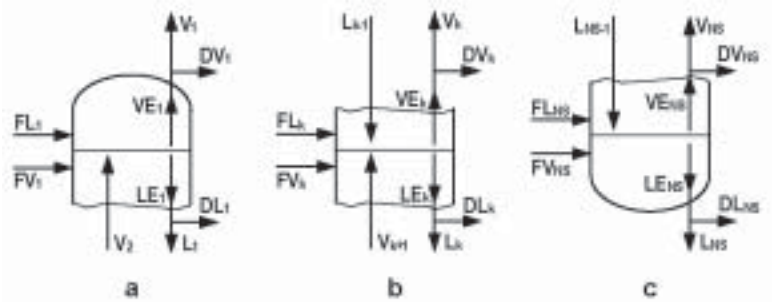

Fig. 2. Column streams: a- column top, b- a tray inside the column, c- column bottom

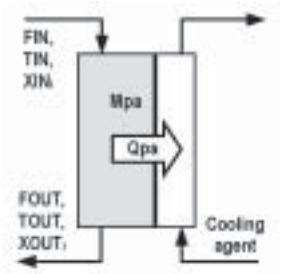

Fig. 3. Pumparound diagram

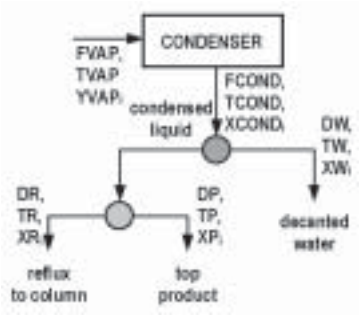

Fig. 4. The condenser with tank

Summation condition:

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

Phase equilibrium:

$$0 = Y_{NS,i} - K_{NS,i} \cdot X_{NS,i} \quad i = 1,...,NC \tag{21}$$

Summation condition:

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

Total material balance:

$$\frac{dm_{NS}}{dt} = FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS} - LE_{NS} \tag{23}$$

Energy balance:

$$0 = FL_{NS} \cdot HFL_{NS} + FV_{NS} \cdot HFV_{NS} + L_{NS-1} \cdot HL_{NS-1} - VE_{NS} \cdot HV_{NS} - \\ - HL_{NS} \cdot (FL_{NS} + FV_{NS} + L_{NS-1} - VE_{NS}) - m_{NS} \sum_{i=1}^{NC} HLP_{NS,i} \cdot \frac{dX_{NS,i}}{dt} \tag{24}$$

Liquid and vapor sidedraws:

$$0 = LE_{NS} - DL_{NS} \tag{25}$$

$$0 = L_{NS} \tag{26}$$

$$0 = VE_{NS} - V_{NS} - DV_{NS} \ . \tag{27}$$

In these equations, the enthalpies and liquid-vapor equilibrium constants 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 and Boston-Britt [1, 8].

Some important characteristics of this model must be emphasized:

-The system is non-linear and 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.

-For this differential-algebraic system, the main problem is to determine consistent initial values for the integration (by computing the algebraic variables values which are consistent with the given initial values of the dynamic variables). A special case where this is satisfied represents the column "true" steady state, with practical relevance.

-The transient time has a value in the range of 5…25 h (for industrial units).

-The system dimension is very large and may put memory management problems; thus, some fine dimensional adjustments – but not reductions! – are needed, i.e. observing that only a few trays in the column have external feeds or sidedraws.

The pumparounds

The model for pumparounds (fig. 3) is based on the equation for heat transfer from the cooled product stream to the cooling agent, with unchanged product composition and flow rate:

Heat transfer: $$\frac{Mpa}{FIN} \cdot \frac{d\,TOUT}{dt} = TIN - TOUT - \frac{Qpa}{FIN \cdot c_p} \tag{28}$$

Composition: $$0 = XIN_i - XOUT_i, \quad i = 1,..., NC \tag{29}$$

Flow rate: $$0 = FIN - FOUT \cdot \tag{30}$$

The condenser with accumulation tank

The author of this work adopted here a very robust model, considering the case of a total condenser with "perfect" controlled temperature (as formulated in the equations (32), (39) and (41)) and constant liquid holdup in the tank (the decanted water accumulation is modeled too, assuming the water as pseudo-component "NC"):

Condensed liquid composition:

$$0 = XCOND_i - YVAP_i \quad i = 1,...,NC \tag{31}$$

Condensed liquid temperature:

$$0 = TCOND - TFIX \tag{32}$$

Condensed liquid flow rate:

$$0 = FCOND - FVAP \tag{33}$$

Decanted water flow rate:

$$0 = DW - fw \cdot FCOND \cdot XCOND_{NC} \tag{34}$$

Top product flow rate: $$0 = DP - \frac{FCOND - DW}{1 + RR} \tag{35}$$

Reflux flow rate: $$0 = DR - RR \cdot DP \tag{36}$$

Reflux composition:

$$0 = XR_i - \frac{XCOND_i \cdot FCOND}{FCOND - DW} \quad i = 1,...,NC-1 \tag{37}$$

$$0 = XR_{NC} - \frac{XCOND_{NC} \cdot FCOND - DW}{FCOND - DW} \tag{38}$$

Reflux temperature: $$0 = TR - TCOND \tag{39}$$

Top product composition:

$$0 = XP_i - XR_i \quad i = 1,..., NC \tag{40}$$

Top product temperature: $$0 = TP - TCOND \tag{41}$$

Decanted water composition:

$$0 = XW_i \quad i = 1,..., NC-1 \tag{42}$$

$$0 = XW_{NC} - 1 \tag{43}$$

Decanted water temperature:

$$0 = TW - TCOND \ . \tag{44}$$

Summary of model characteristics

The plant model above is based on standard model formulation for distillation columns. However, some significant changes are made in order to improve the numerical solution:

- The model is explicitly oriented to a topological description of the plant.
- The total material balance equations (5) and (14) and the energy balance equations (6), (15) and (24) have an adapted form, in order to make the system easier to solve.
- A robust and original model for the top total condenser with accumulation tank is included, based only on material balance equations instead of equilibrium equations. The author experienced a close to reality system behavior, with lower computational effort than using the equilibrium-based model.

Conclusions

This work presented a "full-scale" dynamic model for the crude oil plant, based on pseudo-components, making use of the MESH equations with some additional simplifications. It leaded to a robust dynamic model, proving reasonable dimensions and a good accuracy, as it will be shown in the second part of this work. The structural/topological approach permits the model integration in any appropriate software environment, in order to simulate the crude oil plant.

$0 = TW - TCOND$

Nomenclature

Molar flow rates:

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

Molar fractions:

XFL, YFV – pseudo-component in liquid/vapor feed;
X, Y – pseudo-component in liquid/vapor on tray;
XIN, XOUT – pseudo-component in product to/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:

T – pseudo-component normal boiling temperature;
TIN, TOUT – product to/from heat exchanger;
TFIX – set point for condensed liquid;
TCOND – condensed liquid;
TW – decanted water;
TP – top product;
TR – reflux to the column.

Molar enthalpies:

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

Others:

K – liquid-vapor equilibrium constant;
m_0 – constant liquid holdup on tray;
m – liquid holdup on tray;
bm – coefficient in the holdup equation;
NS – number of column trays;
NC – number of pseudo-components in crude feed;
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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