Petroleum Fractions Liquid – Vapor Equilibrium Simulation using Unisim Design®

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The Unisim® environment represents a valuable tool applied for chemical process simulation and automatic control systems associated to such processes. Due to the specific nature of petroleum products, instead of pure chemical components the simulator operates with pseudocomponents, with different configuration procedures for each case. If the operation for the first case is well known to the smallest detail, configuring the simulator being straight forward, the second case is more complex and the configuration is carried out by specific operations. The paper describes research carried out in two directions. For the first one, the necessary stages for the usage of pseudocomponents in the computation of liquid-vapor equilibrium. The second stage is represented by the identification and testing of the Unisim® configuration operations for cases in which petroleum products are involved. Three representative cases were analyzed: petroleum, diesel and petroleum – water mixture.

Keywords: Unisim®, chemical process simulation, petroleum products, pseudocomponents

The simulation of chemical processes, especially that of refiery processes and installations, requires as a compulsory step the computation of the liquid – vapor equilibrium, in both transport pipelines, hydraulic resistances, separator vessels as well in fractioning columns. The simulation of chemical processes is possible if numerical sumelators ar used, such as HYSYS, Unisim® and PRO II, each of these solutions including specialized modules for the computation of the liquid – vapor equilibrium of petroleum products.

In the case of the classical usage of the Unisim® simulator, the computation of the liquid – vapor equilibrium is conditioned by following three configuration steps [1]:

- selecting the chemical components from the simulator database;
- selecting the thermodynamic model of the liquid – vapor equilibrium;
- defining the concentrations associated to each chemical component.

This technique is applied only to processes which involve pure chemical components. For exemple, in the case of binary fractioning, the HYSYS simulator was used for static and dynamic simulation fo the fractioning process [2, 3].

Most of the processes in refineries operate with petroleum products, including oil. In these cases the Unisim® simulator will operate with pseudocomponents instead of chemical components [4-6]. The research carried out by the authors indicated the fact that switching from chemical components whose physical properties are included in the simulator database, to pseudocomponents, involves the following stages:

- defining the properties of the petroleum product (PRF distillation curve, STAS distillation curve, average properties);
- generating pseudocomponents in the range of boiling temperatures for the petroleum product;
- selection of pseudocomponents which define a distillation curve as close as possible to the experimental one;
- computing the optimal concentration for each selected pseudocomponent such that both the distillation curve and the average properties are as close as possible to the experimental ones.

This new approach for the usage patterns of the Unisim® simulator requires following different configuration steps of the environment. The paper covers the actual simulator configuration procedure for three fundamental petroleum products:

a) oil;
b) petroleum product (gasoline, diesel);
c) oil – water mixture.

For each of these options, both the configuration particularities of the Unisim® simulator and an application for liquid – vapor equilibrium computation are presented.

Particularities in defining the component list for oil

This case is specific to a petroleum product without being accompanied by pure chemical components. Crude oil belongs to this category. The simulation of liquid – vapor equilibrium requires following the listed steps:

a) selecting the thermodynamic model used by petroleum products;
b) analysis of the petroleum product;
c) introducing in the simulator of the laboratory analysis characteristics of the petroleum product;
d) computing the pseudocomponents;
e) defining the simulation window *Case main;*
f) simulation of the liquid – vapor equilibrium.

Selecting the thermodynamic model

For petroleum products, the usage of the Peng – Robinson thermodynamic model is reccomended. This

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Fraction	Initial [°C]	Final [°C]	Distilled volume [%]	Cummulative volume [%]	d_{15}^{15}
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

Table 1
CRUDE OIL PROPERTIES FOR PROCESSING

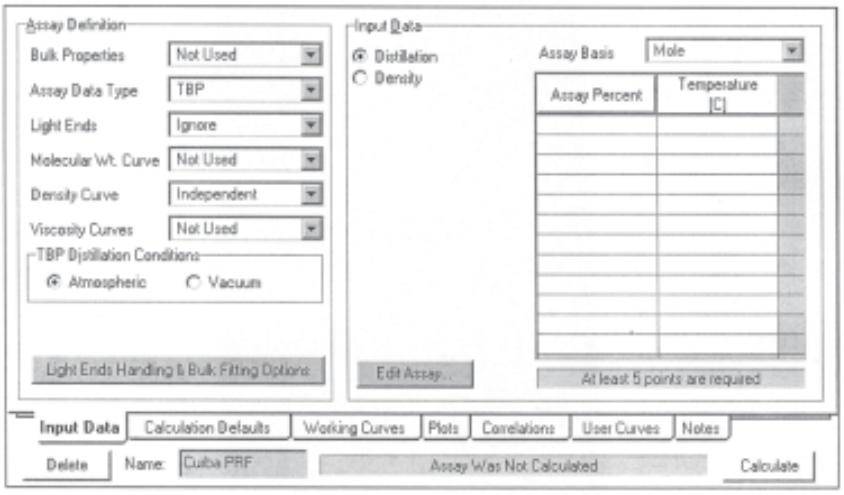


Fig. 1 ***Assay*** window for oil TBP curve definition

model is based on the state equation with the same name, developed in 1976 and respects the following requirements [7, 8]:

a) the equation parameters should be expressed based on the critical properties and the acentric factor of the chemical components;

b) the model should correctly predict the properties in ranges around the critical point;

c) the mixing rules only concern binary mixtures, being temperature and pressure independent;

d) the state equation can be applied to the computation of the hydrocarbon mixture properties.

In the Unisim Design® simulation environment the selection of the thermodynamic model is performed with the help of the command menu *Current Fluid Package*, where the *Add* command is used to insert the Peng – Robinson thermodynamic model.

Analysis of the petroleum product

The petroleum product corresponding to this category is oil which supplied an atmospheric distillation column. The laboratory data associated to the TBP curve are listed in Table 1 [9]. These analyses contain both the TBP distillation curve as well as the average percentage – density curve.

Inserting the laboratory analyses data of the petroleum product

In order to insert the data resulting from the laboratory analysis in the Unisim Design® simulation environment, the following steps have to be carried out:

a) the Fluid Package window is minimized and we return to the Simulation Basis Manager;

d) the Add command is activated for the definition of the oil used as raw material. Considering the type of laboratory data, in the Assay window the following configuration will be performed (fig. 1):

- Bulk Properties = Not Used
- Assay Data Type = TBP
- Light Ends = Ignore
- Molecular Wt. Curve = Not Used
- Density Curve = Independent
- Viscosity Curves = Not Used

e) For inserting the TBP distillation curve, we select:

-Input Data = Distillation
- Assay Basis = Liquid volume

f) The Edit Assay command is activated and the PRF oil curve is inserted (fig. 2a). At the end of this step, the inserted data is verified, confirmation is done with OK and the program control returns to the Assay window.

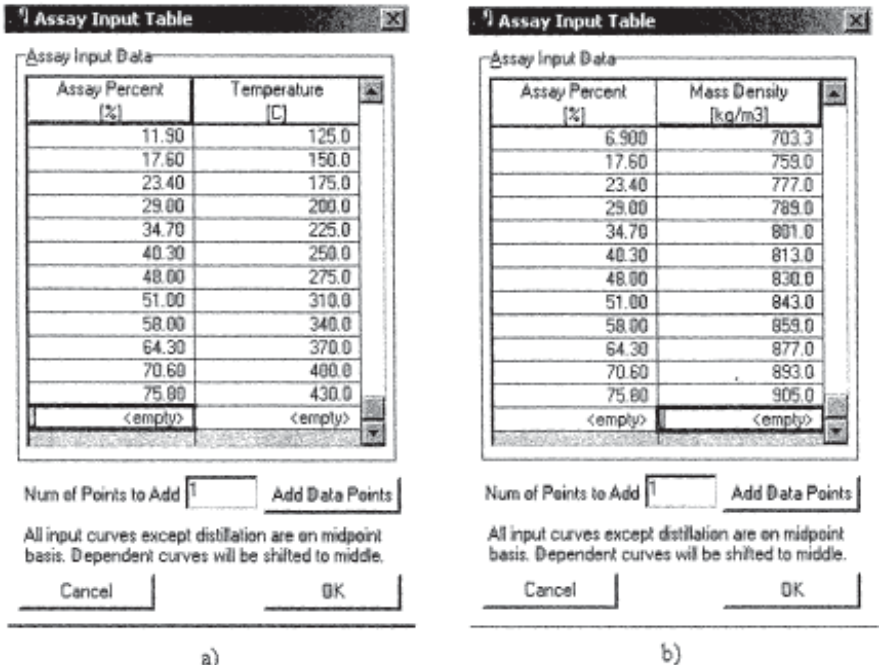


Fig. 2 *Assay Input Table* window for:
a) inserting the TBP distillation curve;
b) inserting the average percentage – density curve

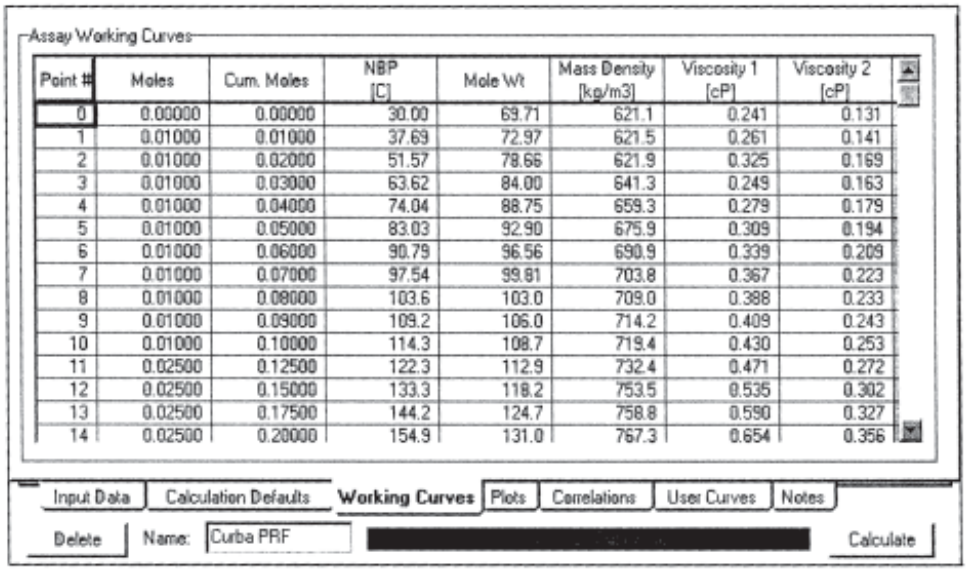


Fig. 3 *Working Curves* window used for viewing the pseudocomponent properties associated to the TBP curve of oil

g) To insert the average percentage – density curve, the option *Input Data* = Distillation option is selected and the command *Edit Assay* is activated.

h) In the new *Input table* window the data corresponding to the average percentage – density curve will be introduced (fig. 2b). At the end of this step, the inserted data is verified, confirmation is done with *OK* and the program control returns to the *Assay* window.

Pseudocomponent computation

Determination of the pseudocomponents takes place in two stages. In the first stage the theoretical pseudocomponents are determined, which correspond to the TBP distillation curve. This stage is implemented by activating the *Calculate* command from the *Assay* window. The result of this mathematical operation can be visualized by means of the command *Working Curves* (fig. 3). In this way, all pseudocomponents ranging from the first to the last distillation temperature are identified.

The second stage contains a computation for determining the concentration of each pseudocomponent so that the TBP curve computed based on the pseudo-components is as close as possible to the experimental one. For this, in the command group *Oil Characterization* from the *Assay* menu the program control is switch to the *Cut/Blend* menu for selection of the pseudocomponents. After performing this operation, the *Add..* button is pushed to edit the TBP curve introduced in this mathematical operation. The mixture which will be selected is called the *Curba PRF* and is available in the *Available Assay* window. This mixture is selected and by pushing the *Add..* button from this menu, the mixture will be specified in the *Oil Flow Information* window (fig. 3). For the pseudo-component selection for this mixture the function *Cut Ranges*, with the option *Auto Cut* can be used (automatic determination of the number of pseudo-components).

As the computation procedure was successful (*Blend Was Calculated*), by means of the *Tables* command the number and properties of the pseudocomponents selected by the simulator are verified (fig. 4). Therefore, for the oil characterized by the PRF curve described in Table 1, the simulation program has identified 40 pseudocomponents. Using the properties and concentrations of each pseudocomponent, the Unisim Design® simulator computes the TBP curve of oil (*Property Plot* function), this curve being compared to the experimental version of the PRF curve (*Composite Plot*), as in figure 5.

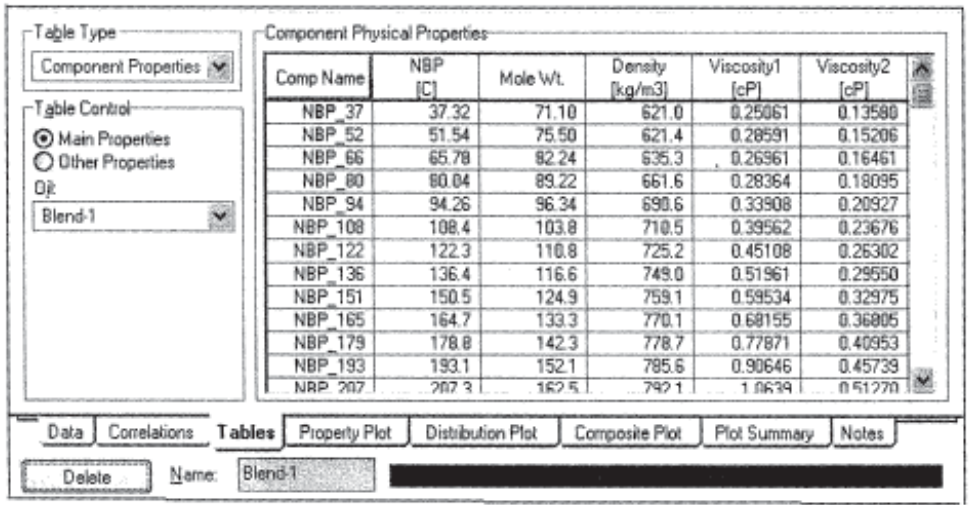


Fig. 4 Physical properties of the pseudocomponents associated to the mixture defined by the PRF curve.

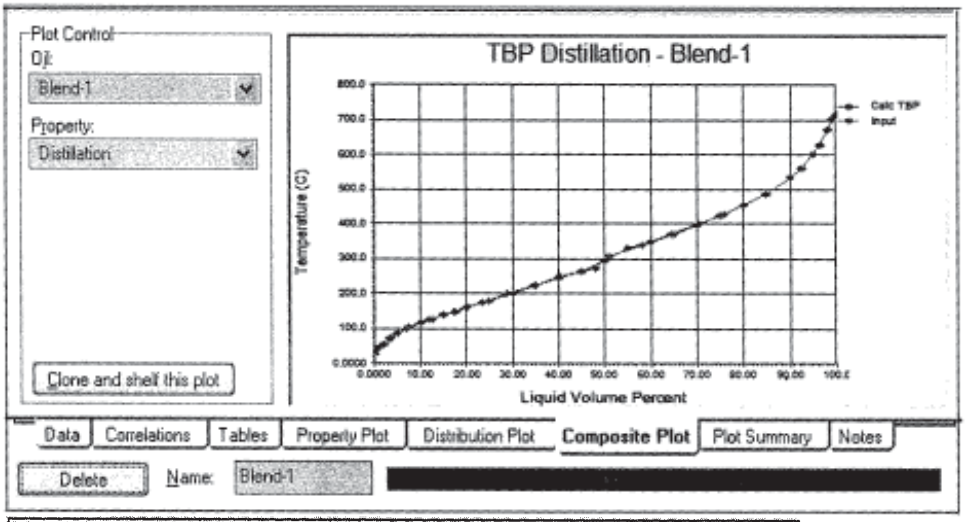


Fig. 5. Comparison between the TBP curve computed based on the pseudocomponents and the experimental curve

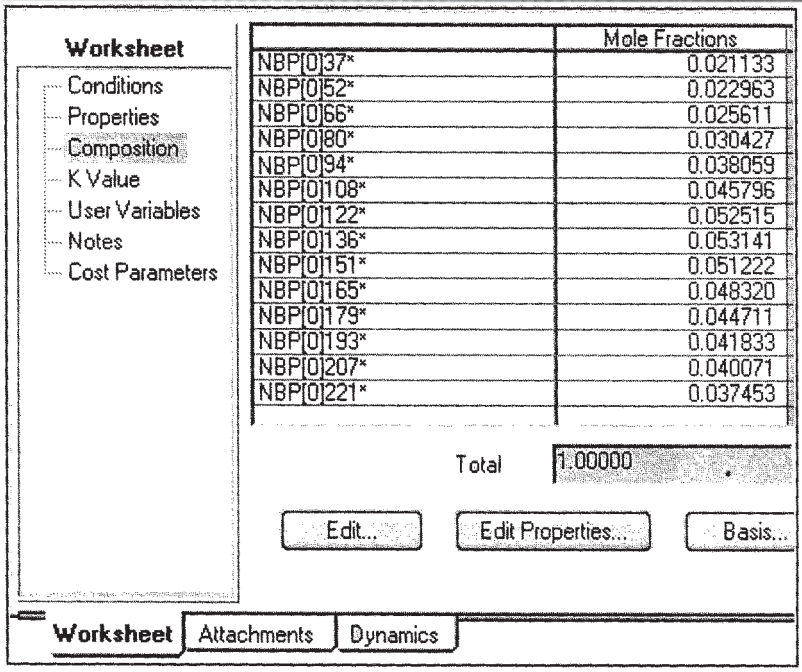


Fig. 6 Pseudocomponent list transferred to the *Master Component List*

Definition of the simulation window

After carrying out the operations concerning the definition of pseudocomponents associated to oil, the command group *Install Oil* from the window *Oil Install Information* will be selected. This command group will load, within the list of chemical components, the pseudocomponents defined for the mixture denoted as *Curba PRF*. The material flux that will use these pseudocomponents will be specified in the *Stream Name* window. For this example the name of the material flux will be *Feed*. Using the command *Return to Basis Environment*, the program control will return to the command menu *Simulation Basis Manager* and the material flux *Feed* becomes active, the user being able to go on to the definition of its properties. The composition of the feeding flux, computed by the simulator, can be

No.	Pressure [bar]	Temperature [°C]	Vaporized fraction [% vol]
1	1	200	40.58
2	2		21.18
3	4		0
4	6		0
5	8		0
6	10		0
7	6	150	0
8		200	0
9		250	7.75
10		300	37.85
11		350	77.35

Table 2
RESULTS CONCERNING THE SIMULATION OF THE LIQUID – VAPOR EQUILIBRIUM FOR OIL AT DIFFERENT PRESSURES AND TEMPERATURES

Table 3
Diesel ASTM distillation curve

Vaporized volume [%]	Temperature [°C]
0	185
16	226
32	246
48	265
54	288
74	310

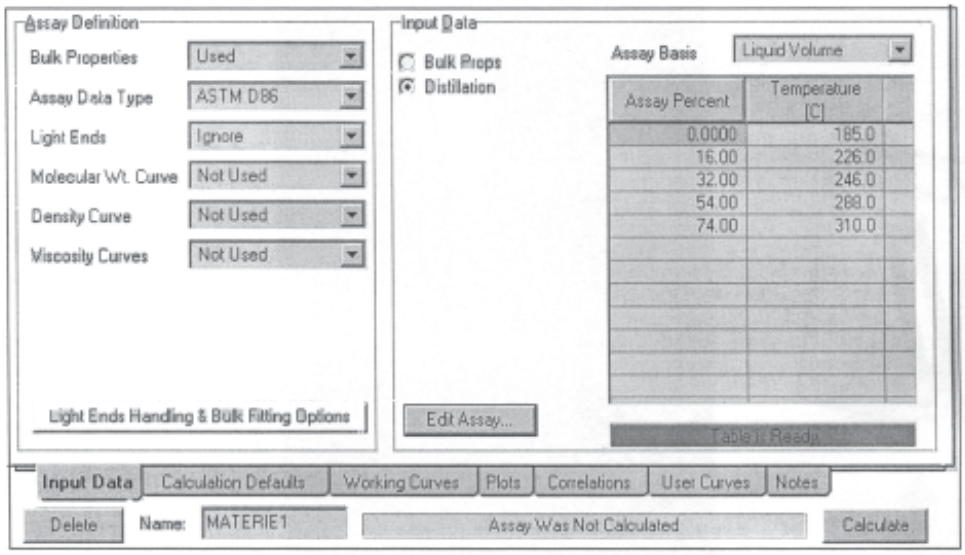


Fig. 7 *Assay* window for inserting the ASTM distillation window

visualized through the command *Composition* from the *Worksheet*, window (fig. 6).

Simulation of the liquid – vapor equilibrium for oil

By means of the newly created program a simulation was carried out for the liquid – vapor equilibrium of the oil characterized by the laboratory analyses defined in table 1. The simulation conditions and results obtained are listed in table 2 [10]. It is thus demonstrated that the increase in pressure reduce the vaporized fraction and the increase in temperature contributes to its growth.

Particularities in the definition of the components list for a petroleum product

This case is specific to a petroleum product, type gasoline or diesel, without this being accompanied by pure chemical components. The petroleum product which was studied is diesel and the simulation of the liquid – vapor equilibrium requires following the same steps as in the case of oil. Subsequently only the particular aspects introduces by the analysis of the petroleum product will be highlighted.

Analysis of the petroleum product

In this case the analyses of the petroleum product are represented by the ASTM distillation curve, values listed in table 3, as well as by mixture properties: density 889.5 kg/m^3 and molecular mass 300 kg/kmol [11].

Introduction of laboratory analyses in the simulator

Compared to the previous case for oil, the laboratory analyses for this petroleum product are less consistent, which is reflected in the way in that these will be specified. For the definition in the UNISIM environment of the ASTM curve for diesel we proceed in the same way like for oil, following the steps defining by the command group Oil Manager and *Oil Characterization*. The *Add* command is activated and in the *Assay* window the following specifications are introduced:

- *Bulk Properties* = USED
- *Assay Data Type* = ASTM D86
- *Light Ends* = Ignore
- *Molecular Wt. Curve* = Not Used
- *Density Curve* = Not Used
- *Viscosity Curves* = Not Used

The *Edit Assay* command is activated and the data associated to the ASTM distillation curve for diesel is inserted (fig. 7). At the end of this operation, the inserted data is checked, they are confirmed with OK and the program control returns to the *Assay* window.

For inserting the data characterizing the mixture properties, in the *Input Data* window the *Bulk Props* option will be activated while specifying the following:

- *Molecular Weight* = 300
- *Standard Density* = 889.5 kg/m^3

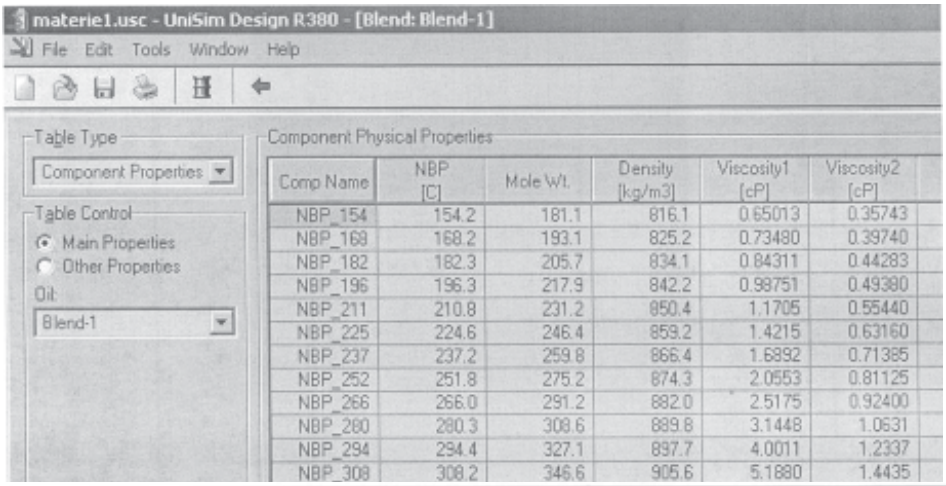


Fig. 8 Physical properties of the pseudocomponents associated to the petroleum product

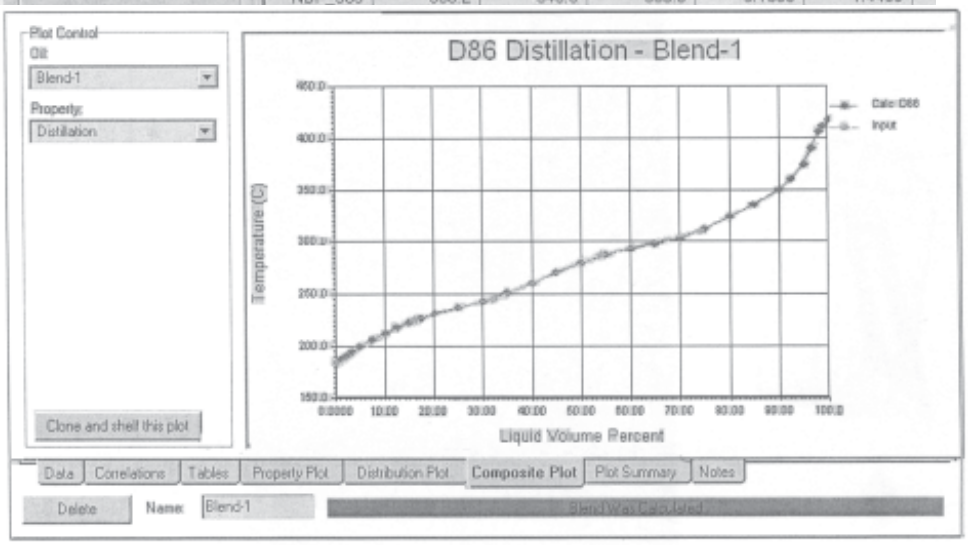


Fig. 9 Comparison between computed and experimental ASTM curve

Computation of the pseudocomponents

Computing of the pseudocomponents associated to the petroleum product is carried out in the same manner as for oil, that is:

a) The *Calculate* command from the Assay window is activated, thus identifying all pseudocomponents between the first and last distillation temperature.

b) In the command group *Oil Characterization* from the *Assay* menu the control of the program is switched to the *Cut/Blend* menu for selecting the pseudocomponents and the *Add*.. command is activated to link-edit the TBP curve to this mathematical operation. The mixture to be selected is called *PRF Curve* and can be found in the *Available Assay* window.

c) To define the pseudocomponents within this mixture, the *Cut Ranges* function is used, with the *Auto Cut* option. If the computation procedure is successful, the number and properties of the selected pseudocomponents will be verified as in figure 8. For the diesel characterized by the ASTM curve described in table 3, the simulation program has identified 23 pseudocomponents. Using the properties of the 23 pseudocomponents, the ASTM curve for diesel is recalculated, the user being able to compare the experimental curve with the computed one (fig. 9).

Defining the simulation window

This operation is performed in a similar way to the one presented before in the case of oil. The concentrations of the pseudocomponents in the diesel flux, computed by the simulator, can be visualized with the help of *Composition* command from the *Worksheet* window (fig. 10).

Simulation of the liquid-vapor equilibrium for diesel

The purpose of the study of liquid – vapor equilibrium for this petroleum product was that of determining if diesel is in liquid or partially vaporized phase, as well as determining diesel properties for the following work conditions:

A.Temperature 340°C and pressure 30 bar (fig. 11a).

B.Temperature 340°C and pressure 60 bar (fig. 11b).

The result shown in figure 11 indicates the fact that the petroleum product is in liquid phase at the mentioned pressures.

Particularities in defining the component list for oil – water mixture

This case is different when compared to the previous ones, requiring a specific approach of the Unisim® simulator configuration. Simulation of the liquid – vapor equilibrium requires following the stages:

a) selection of the thermodynamic model ;

b) analysis of the petroleum product;

c) selection of the pure chemical components;

d) tnserting in the simulation of laboratory analyses of the petroleum product;

e) computation of the pseudocomponents;

f) defining the simulation window;

g) simulation of the liquid – vapor equilibrium.

Selection of the thermodynamic model

The first stage is carried out according to the above-mentioned mechanism. Because the oil coming from the extraction well contains only hydrocarbons and water, the same Peng-Robinson thermodynamic model was selected,

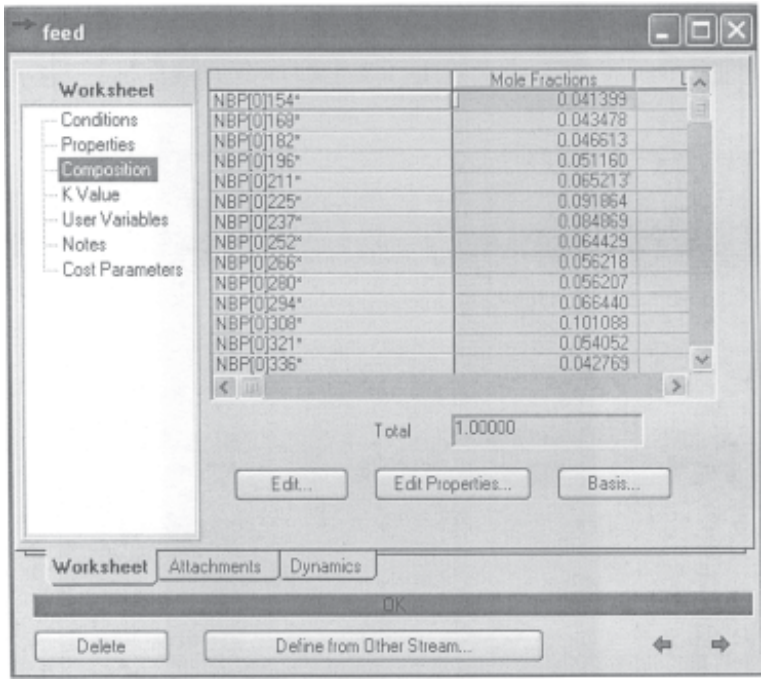


Fig. 10 Components concentration of the diesel petroleum product.

Stream Name	feed	Liquid Phase
Vapour / Phase Fraction	0,000000	1,00000
Temperature [C]	340,000	340,000
Pressure [bar]	30,0000	30,0000
Molar Flow [kgmole/h]	100,000	100,000
Mass Flow [kg/h]	20547,2	20547,2
Std Ideal Liq Vol Flow [m3/h]	24,6036	24,6036
Molar Enthalpy [kcal/kgmole]	-65571,2	-65571,2
Molar Entropy [kJ/kgmole-C]	682,365	682,365
Heat Flow [kcal/h]	-6,55712e+006	-6,55712e+006
Liq Vol Flow @Std Cond [m3/h]	24,6036	24,6036
Fluid Package	Basis-1	Basis-1

a)

Stream Name	feed	Liquid Phase
Vapour / Phase Fraction	0,000000	1,00000
Temperature [C]	340,000	340,000
Pressure [bar]	60,0000	60,0000
Molar Flow [kgmole/h]	100,000	100,000
Mass Flow [kg/h]	20547,2	20547,2
Std Ideal Liq Vol Flow [m3/h]	24,6036	24,6036
Molar Enthalpy [kcal/kgmole]	-65643,6	-65643,6
Molar Entropy [kJ/kgmole-C]	679,921	679,921
Heat Flow [kcal/h]	-6,56436e+006	-6,56436e+006
Liq Vol Flow @Std Cond [m3/h]	24,6036	24,6036
Fluid Package	Basis-1	Basis-1

b)

Fig. 11 Results for liquid – vapor equilibrium, computed for diesel at: a) 30 bar; b) 60 bar

	Fraction	$T_{initial}$ [°C]	$T_{average}$ [°C]	T_{final} [°C]	Mass [g]	Fraction percentage [% vol]	Cummulated oil fractions [% vol]	Oil and water fractions [% vol]	Density d_4^{20}
Atmosferic	1	82	141	205	38	4.53	4.53	36.53	0.7993
	2	205	219	227	40	4.77	9.30	41.30	0.8451
Vacuum	3	232	240	257	42	5.01	14.31	46.31	0.8591
	4	257	268	280	44	5.25	19.56	51.56	0.8738
	5	280	300	312	44	5.25	24.81	56.81	0.8940
	6	312	324	340	44	5.25	30.06	62.06	0.9051
	7	340	345	345	22	2.65	32.71	64.71	0.9107
Residue					564	67.30	100.00		
TOTAL					838	100.00			

Table 4
RESULTS OBTAINED FOR ATMOSFERIC AND VACUUM DISTILLATION OF THE ANALYZED SAMPLE

which is characteristic to mixtures of non-polar hydrocarbons.

Analysis of the petroleum product

The petroleum product is oil directly extracted from a well, containing 32% water by mass. Through static separation water is eliminated, for the resulting oil an atmosferic and vacuum distillation is performed with the results listed in table 4. Given the fact that distillation of the oil in the laboratory cannot take place in the presence of water, the results obtained for the TBP curve of oil have to be corrected with regard to the distilled volume.

Selection of pure chemical components

In the mixture there is only one pure chemical component, water. To introduce this pure chemical component we proceed as follows:

- In the *Simulation Basis Manager* window the command *Add* is activated, leading to the opening of the command window *Component List* – 1. In the dialog window *Match* and indicator for water is inserted, namely H_2O, and the

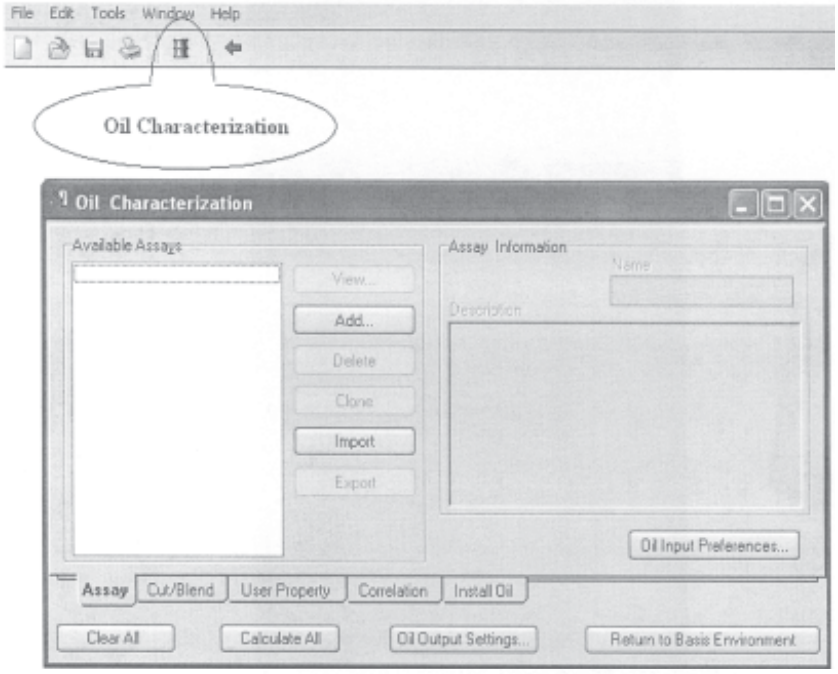


Fig. 12 Activation of the *Oil Characterization* command menu

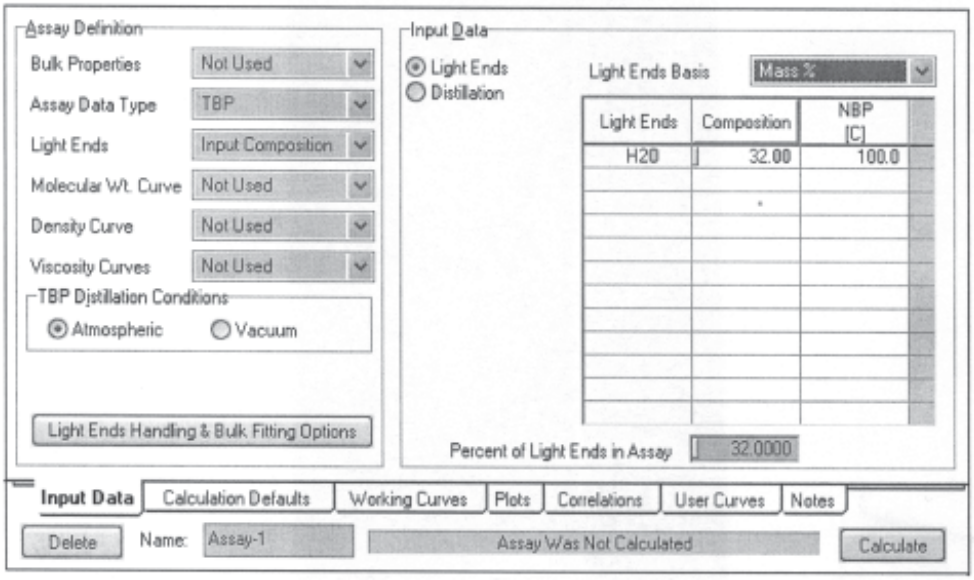


Fig. 13 Specifying water concentration in the water – oil mixture.

Add Pure command is activated. The effect of this command is inserting the pure component water in the list.

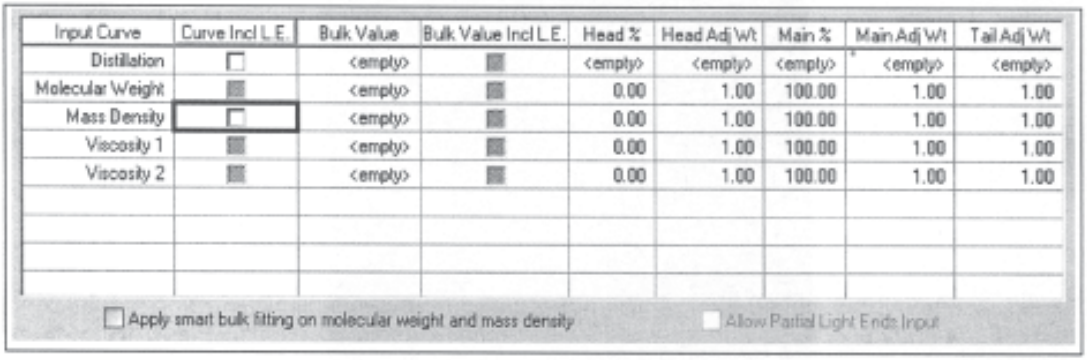
Introduction in the simulator of laboratory analyses of the petroleum product

After inserting water in the component list, the group *Oil Characterization* is activated, performed through the icon from the toolbar of the simulator (fig.12). Within the window the Assay menu is selected and afterwards the *Add* command. By executing this command, the control of the mixture definition operations is transferred to the Assay command window, similarly to the other use cases.

Light or non-petroleum components must be inserted before the definition of the petroleum mixture. To do this the *Assay Data Type* command is activated and the option *TBP* is selected, because laboratory data contains this analysis. In the *Light Ends* dialog window the option *Input Composition* is selected and the corresponding value for the water concentration in the oil-water mixture is inserted, 32% mass (fig. 13).

The analyses of the petroleum product, that is oil without water, include the TBP distillation curve and a curve of physical properties (density – distilled volume), sufficient data for defining in the simulator of the chemical pseudocomponents that are to be used by the simulation. In this case *Bulk Properties* will not be used because the density and viscosity properties are associated only to the petroleum product and do not define the water – oil mixture. For inserting the data which define the TBP distillation curve, the option *Distillation* from the *Input Data* menu is activated and the experimental data is inserted associated to the density – distilled volume curve. Given the fact that water has a lower boiling point than that of the first distilled oil fraction, the distilled volume associated to oil has to be compensated by adding the water volume, namely 32%.

Customizing the specifications for the chemical components continues with the implementation of the link between the water component and the petroleum product. Thus, in the Assay window the command *Light Ends Handling Bulk & Fitting Options* is activated, command which will open a new window in which the user will deactivate the implicit options for the chemical components of the *Light Ends* category, the distillation curve, *Distillation*, and density variation curve, *Mass Density* (fig. 14). These options were initially considered as implicit by the simulator because of the specification inserted through the petroleum product analysis.



Input Curve	Curve Incl L.E.	Bulk Value	Bulk Value Incl L.E.	Head %	Head Adj Wt	Main %	Main Adj Wt	Tail Adj Wt
Distillation	☐	<empty>	■	<empty>	<empty>	<empty>	<empty>	<empty>
Molecular Weight	■	<empty>	■	0.00	1.00	100.00	1.00	1.00
Mass Density	☐	<empty>	■	0.00	1.00	100.00	1.00	1.00
Viscosity 1	■	<empty>	■	0.00	1.00	100.00	1.00	1.00
Viscosity 2	■	<empty>	■	0.00	1.00	100.00	1.00	1.00

☐ Apply smart bulk fitting on molecular weight and mass density ☐ Allow Partial Light Ends Input

Fig. 14 Deactivation the implicit specifications concerning chemical component properties

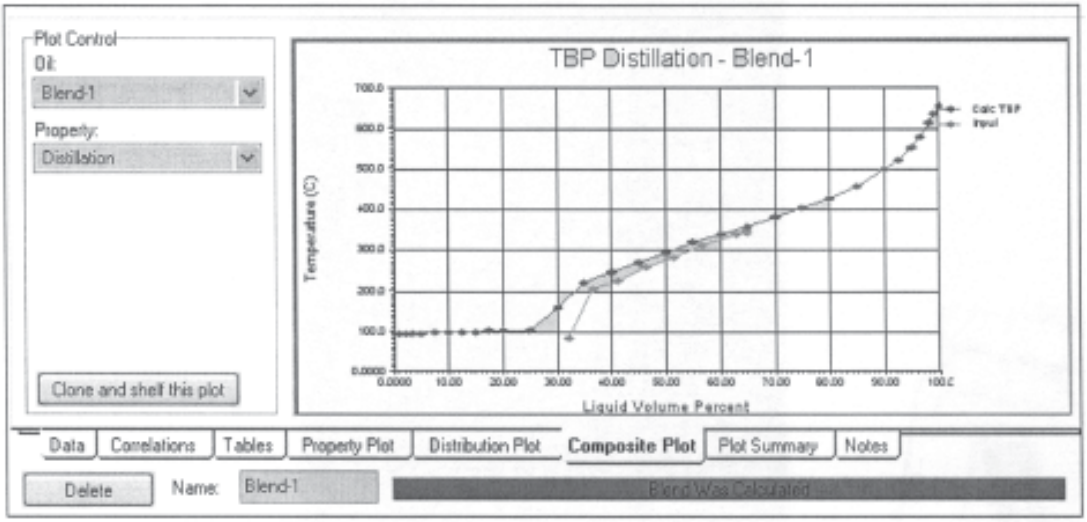


Fig. 15 Comparison between the experimental and computed water – oil mixture TBP curves

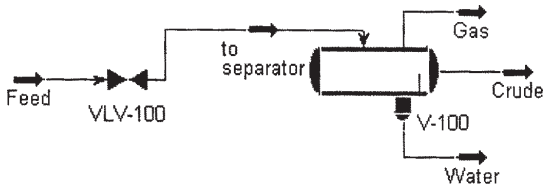


Fig. 16 Simulation diagram associated to a three-phase separator

Computing the pseudocomponents

After carrying out the operations presented until this point, the following step consists in computing the pseudocomponents of the mixture. The computation is activated through the *Calculate* command, existing in the *Assay* command window. The green color obtained in the dialog window signalizes the operation success. Using the *Working Curves* command details are obtained regarding all 50 pseudocomponents computed by the simulator. The first pseudocomponent of the water – oil mixture is similar to water, having the boiling point at 100.3°C. The configuration of the simulator continues with the selection of the command group *Cut/Blend* of the window Oil *Characterization*, activation of the *Add* command, specifying the user-defined mixture, *Assay*, followed again by the *Add* command. The computation mode of the mixture composition is implicitly selected as *Auto Cut.*

Figure 15 illustrates comparatively the TBP curve of the water – oil mixture and the computed curve using the pseudocomponents determined by the simulator. It can be seen that for the first 25& distilled fractions, the boiling point of the pseudocomponents lays around 100°C, reflecting thus the water component. In the interval [25…35] % distilled volume the simulator has introduced pseudocomponents with a boiling point higher than 100°C to create the continuous link between water and oil. This is the distillation range with the highest error. After the point represented by 35% distilled volume, the pseudocomponents calculated by the simulator are very close to the experimental data. Because experimental data does not cover the whole range [0…100] % distilled volume, the simulator has generated a series of pseudocomponents which naturally continue the trend of the oil TBP curve.

Definition of the simulation window

This operation is carried out in a similar manner to the ones presented before for oil and diesel. The concentrations of the pseudocomponents of the water – oil mixture are visualized by means of the *Composition* command of the *Worksheet* window. The result of the operation is shown in table 5.

Simulation of the liquid – vapor equilibrium for water – oil mixture

In oil wells, the water – oil mixture resulting from pumping type wells is processed in three-phase separators, for gas and water removal from the oil. Usually the working temperature is 50°C at 2 bar pressure. For the simulation of the three-phase simulator a simulation program is implemented, using mathematical models available in the Unisim® environment (fig. 16). Using the operating specifications mentioned above, the gas, oil and water fluxes leaving the separator are computed, as well as the composition of these fluxes in table 5.

Component	Feed [mole fraction]	Gas [mole fraction]	Crude oil [mole fraction]	Water [mole fraction]
H_2O	0.766101	0.045382	0.001348	1.000000
NPB[0]106	0.002661	0.054994	0.000112	
NPB[0]119	0.003751	0.077806	0.000089	
NPB[0]133	0.003247	0.067499	0.000041	
NPB[0]147	0.003134	0.065256	0.000009	
NPB[0]162	0.003157	0.065761	0.000006	
NPB[0]176	0.003158	0.065787	0.000003	
NPB[0]192	0.004850	0.101031	0.000004	
NPB[0]206	0.006651	0.138515	0.000015	
NPB[0]219	0.011239	0.231284	0.000735	
NPB[0]233	0.013388	0.084604	0.049528	
NPB[0]248	0.009354	0.001835	0.049200	
NPB[0]263	0.011412	0.000216	0.060536	
NPB[0]276	0.011179	0.000027	0.059348	
NPB[0]291	0.009203	0.000003	0.048866	
NPB[0]305	0.009442		0.050133	
NPB[0]320	0.011137		0.059132	
NPB[0]334	0.014363		0.076261	
NPB[0]347	0.013654		0.072500	
NPB[0]362	0.010015		0.053178	
NPB[0]377	0.009946		0.052812	
NPB[0]391	0.009378		0.049796	
NPB[0]405	0.008360		0.044391	
NPB[0]420	0.007841		0.041635	
NPB[0]438	0.011309		0.060049	
NPB[0]468	0.008600		0.045665	
NPB[0]496	0.007772		0.041265	
NPB[0]521	0.005235		0.027798	
NPB[0]552	0.003496		0.018563	
NPB[0]578	0.002655		0.014096	
NPB[0]606	0.001635		0.008682	
NPB[0]634	0.001101		0.005848	
NPB[0]676	0.001574		0.008356	

Table 5
FLUX COMPOSITION FOR THE THREE-PHASE SEPARATOR

Conclusions

The Unisim® simulation environment is applied to the simulation of chemical processes and automatic control system associated to these processes. The specific nature of petroleum products makes the simulator to operate with pseudocomponents. During the research carried out by the authors, the following steps were highlighte for pseudocomponent definition:

a) defining the properties of the petroleum product (PRF distillation curve, STAS distillation curve, average properties);

b) generation of pseudocomponents in the range of boiling points for the petroleum product;

c)Automatic selection of pseudocomponents which define a distillation curve as close as possible to the experimental one;

d) computing the optimal concentration of each selected pseudocomponent such that both the distillation curve and the average properties are as close as possible to the experimental ones.

The paper presented details regarding configuration operations of the Unisim® environment for cases in which petroleum products are involved: oil, diesel and oil – water mixture. For each of these use cases applications are described for liquid – vapor equilibrium which represent initial elements for simulating the specific chemical processes in oil refining.

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