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USE OF GENETIC ALGORITHMS IN CREATING OIL BLENDS REQUIRED FOR REFINERY DISTILLATION PLAN

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ABSTRACT

In Romania, the oil refineries were designed to process the crude oil extracted from the deposits located in their immediate vicinity (Suplacu de Barcău Refinery, 1 Mai Refinery, Câmpina Refinery, Vega Refinery and Dărmănești Refinery), to process crude oil imported from external oil basins (Onești Refinery, Brazi Refinery, Teleajen Refinery, Midia Refinery and Pitești Refinery) and to process crude oil from the Muntenia and Oltenia oil basins (Brazi Refinery and Pitești refinery).

The closing of some refineries after 1990, the reduction of crude oil imports and especially the tightening of the quality conditions of the delivered petroleum products (the need to reduce the sulphur content of petroleum products, the use of bio-fuels) led to the reconsideration of deliveries to the refineries that remained in operation, through the creation of mixtures of crude oils extracted from Romania (for the Brazi Refinery) and the import of crude oil mixtures for the Teleajen and Midia Refineries, which would ensure the new quality conditions of finished petroleum products.

The article describe how to create crude oil blends according to refinery requirements, using both classical estimation methods and genetic algorithms to determine the variation in the properties of these blends.

Keywords: mixtures, genetic algorithms, crude oil, properties.

INTRODUCTION

Usually, refineries are created to process a certain type of crude oil. But at some point, in the refinery's activity, problems may arise in the supply of crude oil due to the change in the political situation of the supplier or the change in its price.

The first time when the problem of creating crude oil blends was raised was at the beginning of 1979, when Iran stopped the supply of crude oil to countries that did not accept the new state order (Islamic republic) [1].

Romania was the first affected by this decision because the refineries that were being built at the time (Onești, Midia and Brazi) had to change their crude oil supplier, asking Russia to create a product similar to Iranian crude oil (REBCO) [2].

Also, after 1990, the refining of crude oil extracted from Romanian oil fields was affected by [3]:

a. Reducing the rate of discovery of new conventional crude oil deposits,
b. Increasing the natural decline of existing deposits (decrease in crude oil production during exploitation),
c. The advance of the water front in the deposit as a result of the decrease in gas pressure and therefore the increase in the water-crude oil ratio during extraction,
d. The increase in the demand for natural gas and therefore the abandonment of the primary extraction of crude oil,
e. Tightening the legislative conditions imposed on fossil fuels (reduction of sulphur content, the need to ensure a minimum of 5% fuel from renewable sources, increasing demand for cars driven by electric motors, etc.),
f. Changing the geo-politics of oil exporting countries in ensuring deliveries to politically and financially approved beneficiaries by them.

Refineries in Romania were designed to process crude oil from the deposits located in their area of activity (a certain type of crude oil and as a result specific oil products result, from the Oltenia and Muntenia oil basins, where the crude oils were mixed before refining and imported in the form of mixtures from other external pools [4].

The types of crude oil processed in Romanian refineries and their qualities are shown in Table 1.

In the conditions of the fluctuation of the price of crude oil on the international market and the need to maintain sales prices of petroleum products at a constant level, any refinery ensures its processing efficiency by [5]:

a. Reducing the profit margin of the refining process,
b. Ensuring cheaper crude oils for processing,
c. Ensuring blended crude oils, similar in quality to the one that was the basis of the refinery design,
d. Creation of a crude oil Blend to ensure petroleum products consistent with market requirements.

Since most of the small refineries that processed crude oil extracted from Romanian oil fields have closed, the Brazi Refinery has to secure a medium-light blend crude oil from crude oil extracted from domestic fields in Romania.

The disappearance of the supply route from Iran and the war between Russia and Ukraine also the need to create a medium crude oil for the Teleajen refinery and a medium-light crude oil for the Midia refinery of the Kazakhstan operating area.

Table 1. Types of crude oil processed in Romania refinery

Refinery	Oil type	Density (kg/dm^3)	Viscosity (cSt)	Pour point (°Celsius)	Sulfur content (%)	Amount processed t/day	Refinery status
Midia	Hard Oil, Iran	0,871-0,877	8,3	-15	1,9	15000	function
Teleajen	Iran light, Iran	0,855-0,860	7,58	-16	1,6	7500	function
Teleajen Engine Oil Block	Light oil	0,8406	3,75	+1	0,18.	1000	close
9 May	Băicoi	0,8483	8,93	+1	0,8	1200	close
Brazi	Heavy oil	0,8537	8,93	+1	1,18	10000	function
Pitești	REBCO-Russia	0,8677	8,3	-8	1,8	15000	close
1 May	Medium oil	0,8804	32,85	-45	0,2.	2000	close
Câmpina	Medium oil	0,8497	6,81	-30	0,2	600	close
Suplacu de Barcău	Suplac hard oil	0,950	6338	-15	1	1000	close
Dărmănești	Medium oil	0,8700	19,14	+15	0,2	1000	close
Onești	REBCO-Rusia	0,8705	7,58	-7	1,2	7500	close

The need to create blend-type crude oils is dictated by [6]:

a. Ensuring a constant volume of oil with strict conditions regarding the physico-chemical properties (to obtain the maximum of quality finished products within the refinery), considering that during the production of the field (which was the basis of the refinery design) both the quantity as well as the quality of the crude oil produced it decreases due to its decline,
b. Ensuring a crude oil with better qualities and therefore higher prices for the sale of finished products,
c. Obtaining better quality finished products (considering that fuel oil has a decreasing sales trend).

At the same time, the oil industry operators operating in Romania have as objectives for the period 2022-2030 [7]:

- Obtaining finished products from renewable sources,
- The maximum reduction of greenhouse effect emissions,
- Increasing the amount of gas extracted from deposits (up to 70% of exploited petroleum fluids),
- Improving the quality of finished products, through the use of stabilizing additives and especially the use of aromatic hydrocarbons.

So, in conclusion we can say that the production of blended crude oils has the following effect:

a. Change in physical properties (density, viscosity, freezing point, pour point),
b. Modifying their processability (white product content, sulphur content, amount of fuel oil, etc.),
c. Modification of the delivery price of finished products.

MATHEMATICAL MODELS REQUIRED FOR PREDICTION OF PROPERTIES OF LIQUID MIXTURES

In the creation of crude oil blends, constant knowledge of the physical properties of both the components and the final product is required.

In practice, blended crudes are formed depending on the end product requirements (i.e. from the interpretation of the distillation curve) and quality conditions (sulphur and paraffin content, etc.).

That is precisely why, after knowing the quality data of the final product, mixtures of two or more crude oils are made in the laboratory and mixtures are made in different proportions, which are later analyzed.

Mathematical relations are also used to predict the properties of the final mixture, depending on the quantities of components that make up the mixture.

To estimate the mixture density of a Blend crude oil, an empirical equation called Kay's mixing rule [8] is used:

$$\rho = \rho_1 x_1 + \rho_2 x_2, \qquad (1)$$

Where ρ is the density of the mixture, ρ_i is the density of component i in the mixture and x_i represents the mole, mass or volume fraction of component i in the mixture.

To estimate the viscosity, the Grunberg-Nissan equation [9] is most often used:

$$\ln \eta = \nu_1 \ln \eta_1 + \nu_2 \ln \eta_2 + \nu_1 \nu_2 G_{12} \qquad (2)$$

In equation 2, η represents the viscosity of the mixture, ν_i and η_i are the volume fraction and viscosity of component i, respectively, and G_{12} is an interaction parameter.

Relation 2 was simplified by Allen [10] by eliminating the interaction parameter G_{12}, the error in the prediction of biodiesel-diesel, diesel-toluene, diesel-benzene mixtures, being between 0.12 and 4.24%.

In the specialized literature, prediction equations were written for the determination of the yield point, the most common equation being written by Rushang and Michael [11], with calculation errors between 0.10 and 0.96 % for mixtures of biodiesel-diesel, diesel-toluene and diesel-benzene mixtures.

The equation of the flow temperature (pure point) T (K) as a function of the volume fraction of a component in the mixture V_B(%), is:

$$T = 253{,}9 + 0{,}1865\ V_B + 0{,}000335\ V_B^2 \qquad (3)$$

In the case of determining the flash point of the mixture, Kay's rule was used, namely:

$$T_{mixture} = \sum_{i=1}^{k} y_i T_i \quad (4)$$

Where $T_{mixture}$ represents the flammability point of a mixture consisting of components that have the flammability point T_i and participate in the formation of the mixture with the volume fraction y_i.

But it is noted that no mathematical equations have been written for the prediction of the distillation point and sulphur content of the mixture.

EXPERIMENTAL SECTION

In order to evaluate the prediction models and write a numerical model based on artificial intelligence, the physical properties of a mixture consisting of two crude oils were determined in the laboratory (Table 2 and Table 3).

The density was determined according to the SR EN ISO 12185 standard - OIL AND PETROLEUM PRODUCTS - Determination of density. U-oscillating tube method,

The flash point was obtained according to the SR EN ISO 2719 standard – PETROLEUM PRODUCTS – Pensky – Martens closed vessel method,

Also, the kinematic and dynamic viscosity were determined according to the SR EN ISO 3104/AC:09 standard – PETROLEUM PRODUCTS – Opaque and transparent liquids

The sulphur content of the crude oil and the distillation characteristics at atmospheric pressure of the mixture of crude oils were determined according to the standards SR EN ISO 20846:12 – PETROLEUM PRODUCTS – Ultraviolet fluorescence method and SR EN ISO 3405:11 – Petroleum products.

Table 2. Physical properties of oil analyzed

Oil/Parameters	**Oil 1**	**Oil 2**
Flash point, °C (Pensky – Martens)	60	45
Sulphur, mg/kg	5,5	15,9
Density at 15°C, kg/m^3	834,3	836,8
Density at 20°C, kg/m^3	831,2	833,4
Kinematic viscosity la 40 °C, mm^2/s	2,4379	2,5399
Kinematic viscosity la 20 °C, mm^2/s	3,7971	4,1593
Distillation curve:		
Initial point, °C	164	177
10%(v/v), °C	195	198
20%(v/v), °C	215	225
30%(v/v), °C	232	235
40%(v/v), °C	247	250
50%(v/v), °C	259	265
60%(v/v), °C	272	279
70%(v/v), °C	286	295
80%(v/v), °C	300	310
90%(v/v), °C	318	330
Final boiling point, °C	346	355
- %(v/v) recovered at 250 °C,	43	40
- %(v/v) recovered at 350 °C,	98	97
- 95 %(v/v), recovered at,°C	334	344

Table 3. Physical properties of blend oil analyzed

Parameters	**Oil 1 = 20% Oil 2 = 80%**	**Oil 1 = 50% Oil 2 = 50%**	**Oil 1 = 80% Oil 2 = 20%**
Flash point, °C (Pensky – Martens)	48	52	57
Sulphur, mg/kg	12,9	10,4	7,6
Density at 15°C, kg/m^3	836,5	835,8	834,7
Density at 20°C, kg/m^3	833,0	832,3	831,5
Kinematic viscosity la 40 °C, mm^2/s	2,5177	2,4883	2,4598
Kinematic viscosity la 20 °C, mm^2/s	4,1404	4,1139	3,8012
Distillation curve:			
Initial point, °C	176	173	170
10%(v/v), °C	206	204	203
20%(v/v), °C	224	221	220
30%(v/v), °C	239	238	238
40%(v/v), °C	254	252	250
50%(v/v), °C	267	265	264
60%(v/v), °C	280	278	276
70%(v/v), °C	295	292	290
80%(v/v), °C	310	307	304
90%(v/v), °C	328	325	323
Final boiling point, °C	355	352	349
- %(v/v) recovered at 250 °C,	37	39	40
- %(v/v) recovered at 350 °C,	97	98	-
- 95 %(v/v), recovered at,°C	343	339	337

The models will be evaluated based on the following statistical indicators:

- EA standard deviation

$$SD = \left(\frac{\sum_{i=1}^{N}(P_{exp,i}-P_{calc,i})^2}{N-m}\right)^{1/2} \quad (5)$$

In relation 5, P_{exp} is the experimentally determined property value and P_{calc} is the computationally determined property value.

Relative mean deviation:

$$ARD\ (\%) = \frac{100}{N}\sum_{i=1}^{N}\frac{|P_{exp,i}-P_{calc,i}|}{P_{calc,i}} \quad (6)$$

Where N represents the number of experiments, m is the number of model parameters, P_{exp} is the value of the analyzed property determined experimentally and P_{calc} the value of the analyzed property determined by calculation.

RESULT AND DISCUSION

In the first part, the values of the physical properties of the mixture (density, viscosity, sulphur content, flash point) were determined based on equations 1, 2 and 4.

The ARD and SD values were also determined (Table 4 and Table 5).

Table 4. ARD values for predictive models of the crude oil blend obtained from the compositions in Table 2

Oil/Parameters	Oil 1	Oil 1 = 20% Oil 2 = 80%	Oil 1 = 50% Oil 2 = 50%	Oil 1 = 80% Oil 2 = 20%	Oil 2
Flash point, °C (Pensky – Martens)	0	0	0,47	0	0
Sulphur, mg/kg	0	0,15	1,40	3,32	0
Density at 15°C, kg/m^3	0	0,005	0,01	0,01	0
Density at 20°C, kg/m^3	0	0,0008	0	0,002	0
Kinematic viscosity la 40 °C, mm^2/s	210	367	418	562	119
Kinematic viscosity la 20 °C, mm^2/s	222	816	648	690	48

Table 5. SD values for predictive models of the crude oil blend obtained from the compositions in table 2

Oil/Parameters	Oil 1	Oil 1 = 20% Oil 2 = 80%	Oil 1 = 50% Oil 2 = 50%	Oil 1 = 80% Oil 2 = 20%	Oil 2
Flash point, °C (Pensky – Martens)	0	0	0,5	0	0
Sulphur, mg/kg	0	0,02	0,30	0,92	0
Density at 15°C, kg/m^3	0	0,10	0,25	0,20	0
Density at 20°C, kg/m^3	0	0,14	0	0,04	0
Kinematic viscosity la 40 °C, mm^2/s	0,83	0,79	0,81	0,84	0,82
Kinematic viscosity la 20 °C, mm^2/s	1,36	1,25	1,31	1,31	1,35

In order to determine the mixture values of the components of a blend type crude oil, a model based on genetic algorithms was proposed in what follows.

In principle, the method inspired by Darwin's theory starts from the definition of a candidate population, which evolves and adapts to the environment to be optimized.

The genotype undergoes changes following a change in the values (mutation) of a component (individual) or following the recombination (mixing) of two individuals (components).

In research practice, the principle of survival of the fitness is applied, that is, the most optimal solution will be chosen (survival of the best individuals).

The model we developed starts from the definition of input data (20 values according to Tables 2 and 3), 20 equations (which describe the evolution of the system) and a maximum of 20 final results (the physical properties of the final mixture).

The equations describing the genetic model are shown in table 6.

Table 6. Equation of genetic algorithms blend oil function by oil ration (first oil X)

Y values	Equation	R^2
Flash point, °C (Pensky – Martens)	$y = -2E\text{-}07x^4 + 4E\text{-}05x^3 - 0{,}0026x^2 + 0{,}1856x + 45$	1
Sulphur, mg/kg	$y = 2E\text{-}07x^4 - 5E\text{-}05x^3 + 0{,}0038x^2 - 0{,}2097x + 15{,}9$	1
Density at 15°C, kg/m^3	$y = 8E\text{-}08x^4 - 1E\text{-}05x^3 + 0{,}0004x^2 - 0{,}0185x + 836{,}8$	1
Density at 20°C, kg/m^3	$y = 3E\text{-}08x^4 - 5E\text{-}06x^3 + 0{,}0002x^2 - 0{,}0213x + 833{,}4$	1
Kinematic viscosity la 40 °C, mm^2/s	$y = 7E\text{-}08x^4 - 1E\text{-}05x^3 + 0{,}0006x^2 - 0{,}0082x + 4{,}1593$	1
Kinematic viscosity la 20 °C, mm^2/s	$y = -2E\text{-}10x^4 - 2E\text{-}09x^3 + 3E\text{-}06x^2 - 0{,}0012x + 2{,}5399$	1
Distillation curve: Initial point, °C	$y = -6E\text{-}07x^4 + 0{,}0001x^3 - 0{,}006x^2 + 0{,}0325x + 177$	1
10%(v/v), °C	$y = -2E\text{-}06x^4 + 0{,}0005x^3 - 0{,}0327x^2 + 0{,}8881x + 198$	1
20%(v/v), °C	$y = -9E\text{-}07x^4 + 0{,}0002x^3 - 0{,}0091x^2 + 0{,}0719x + 225$	1
30%(v/v), °C	$y = -1E\text{-}06x^4 + 0{,}0003x^3 - 0{,}019x^2 + 0{,}4764x + 235$	1
40%(v/v), °C	$y = -9E\text{-}07x^4 + 0{,}0002x^3 - 0{,}0158x^2 + 0{,}4433x + 250$	1
50%(v/v), °C	$y = -1E\text{-}06x^4 + 0{,}0002x^3 - 0{,}014x^2 + 0{,}3031x + 265$	1
60%(v/v), °C	$y = -7E\text{-}07x^4 + 0{,}0001x^3 - 0{,}009x^2 + 0{,}1297x + 295$	1
70%(v/v), °C	$y = -6E\text{-}07x^4 + 0{,}0001x^3 - 0{,}0085x^2 + 0{,}1758x + 279$	1
80%(v/v), °C	$y = -5E\text{-}07x^4 + 0{,}0001x^3 - 0{,}0071x^2 + 0{,}105x + 310$	1
90%(v/v), °C	$y = -6E\text{-}07x^4 + 1E\text{-}04x^3 - 0{,}0044x^2 - 0{,}0453x + 330$	1
- 95 %(v/v), recovered at,°C	$y = -7E\text{-}07x^4 + 0{,}0001x^3 - 0{,}0087x^2 + 0{,}0736x + 344$	1
Final boiling point, °C	$y = -4E\text{-}07x^4 + 8E\text{-}05x^3 - 0{,}0062x^2 + 0{,}095x + 355$	1
%(v/v) recovered at 250 °C	$y = 1E\text{-}06x^4 - 0{,}0002x^3 + 0{,}015x^2 - 0{,}3756x + 40$	1
%(v/v) recovered at 350 °C	$y = 2E\text{-}07x^4 - 5E\text{-}05x^3 + 0{,}0032x^2 - 0{,}0464x + 97$	1

CONCLUSION

The values obtained for the SD and ARD of the properties calculated with the prediction equations mentioned above, give calculation errors compared to the experimentally determined values of a maximum of 0.5% (flash point), 3.32 for the sulphur content, 0.14 for density determined at 15° C and 0.014 to the density determined at 20°C.

But the values determined for the viscosity have a calculation error of more than 8%, which makes this prediction equation not useful.

Numerical models based on prediction equations in the case of their use in the creation of crude oil blends, in order to determine their physical properties, are dictated by errors due to:

a. The presence of paraffins in the crude oil composition, which affects the density determined at 15ºC,
b. The fact that the viscosity of crude oil is difficult to be defined by a numerical model (because of the solution that forms this product-paraffins, waxes, water, sulphur, salts, etc.).

The model created in this material, which is based on the use of genetic algorithms, is more useful to use.

This optimized 20-equation model is very easy to use because:

a. The error is close to the value 0,
b. Values of the physical properties are obtained depending on the composition in a component, at any moment of the formation of the blend,
c. Blends can be created depending on a certain property,
d. The genetic model is constantly optimized.

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