Dewaxing models digitalization in the mathematical model of winter diesel fuel production

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Abstract. The climatic features of Russia, as well as the need for the development of the Arctic and the Great Northern Sea Route, require an increase in the production of winter diesel fuel. The object of the study is obtaining winter diesel fuel. The subject of the study is digitalizing oil-refining processes by building the mathematical model of winter diesel fuel production for the case of combining dewaxing regimes taking into account the logistical aspect. Main research methods: retrospective data analysis, synthesis, comparison, optimization theory methods. A literary review was carried out, the main methods for improving the low-temperature properties of winter diesel fuel were revealed. Study hypothesis: a combination of dewaxing regimes will increase the yield of denormalized and, accordingly, winter diesel fuel. The authors for each mode of dewaxing compiled a mathematical model. Then, the authors constructed a mathematical model of obtaining winter diesel fuel for a combination of dewaxing regimes and taking into account the logistical aspect. The obtained mathematical model can be used to obtain the required amount of winter diesel fuel with compliance with quality requirements and taking into account the logistical aspect.

1 Introduction

Please Relevance. Russia is a country of Hyperborean. Taking into account Russia's large-scale plans for the development of both the Great Northern Sea Route and the Arctic, the need for WDF will only increase. Consequently, low temperatures require winter and arctic diesel fuels. Since 2014 in the Russian Federation, GOST R 55475-2013 "Winter diesel and arctic dewaxed fuel" is in force, which determines the values of the main indicators of WDF [1]. The main indicators are as follows:

1. WDF cloud point. At this temperature, n-alkanes (hydrocarbons with the homologous formula C_nH_{2n+2} , having a linear structure) form crystals. Outwardly, it looks like a turbidity of WDF.

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2. The limiting filterability temperature (hereinafter referred to as LFT). At this temperature, the crystals of n-alkanes become more than 45 microns in diameter [2].

To reduce the cloud point and LFT, it is required to remove n-alkanes C18+ from the diesel fraction and minimize the content of n-alkanes C10-17. The presence of alkanes in winter diesel fuel increases the cloud point, filterability point, and solidification point. Winter diesel fuel with a high content of n-alkanes ceases to meet its purpose, it loses its mobility and cannot enter the combustion chamber of a diesel engine in the right volume and in the right mixture with air. Thus, the dewaxing process (removal of the aforementioned n-alkanes) is key in the production of WDF.

The basic methods for dewaxing are well known. The following methods can be named. Cooling of the feedstock directly for the subsequent extraction of higher n-alkanes. It is also possible to cool the raw material by mixing it with certain solvents (exothermic reaction, that is, requiring the attraction of heat). Cleavage of higher n-alkanes by means of a catalyst to n-alkanes with short chains, and, accordingly, with lower pour points. You can use adsorption to separate the feedstock into components boiling at high temperatures and components, boiling at low temperatures. It should be noted that selective solvents are often used for dewaxing raw materials.

The dewaxing unit can operate in several modes. In this case, the selection coefficients of the normalizer change. That is, each technological mode of operation of the dewaxing unit corresponds to a certain yield factor of the denormalize of interest to us. The problem is to find the optimal combination of dewaxing regimes in order to obtain the maximum amount of the normalizer since at the next stage (compounding) the denormalize is the main component for obtaining WDF. The complexity of this problem leads to the need for digitalization of its solving by building a corresponding mathematical model since full-scale experiments will be expensive for the owner of the refinery.

Hence, we should build the mathematical model for obtaining WDF taking into account the combination of dewaxing modes (hereinafter referred to as MMWDFd). Correct MMWDFd will allow you to get the largest number of WDF in compliance with the required quality indicators.

Therefore, the object of this study is producing winter diesel fuel. The subject of the investigation is digitalizing oil-refining processes by building the mathematical model of producing WDF in combining dewaxing modes. And the purpose of the study is to propose a mathematical model for obtaining WDF by combining dewaxing modes.

2 Materials and Methods

In [3], the researcher preliminarily builds a mathematical model of dewaxing with the use of a catalyst, then attempts to calibrate the obtained mathematical model, taking into account the realities of the production of winter diesel fuel at an industrial plant.

In [4], researchers also consider the process of catalytic dewaxing, propose a mathematical model, and in this mathematical model, the factors of nonstationarity are already taken into account. Taking into account nonstationarity undoubtedly brings the theory of catalytic dewaxing to a new level of quality.

In [5], researchers apply a mathematical model of catalytic dewaxing in relation to heavy and straight-run gas oils in the "reactor-stabilizer column" system.

In [6], researchers compiled a mathematical model of catalytic dewaxing to identify reserves for increasing the yield of denormalize.

In [7], researchers asked how a change in the technological regime affects the dewaxing process and maximizing the denormalize yield. For this, the corresponding mathematical model was also built.

In [8], the researchers thoroughly analyzed the question of whether it is possible to increase the yield of denormalizate in the process of dewaxing the middle distillate fraction by redistributing hydrogen-containing gas between blocks of an industrial plant. The middle distillate fraction is one of the results of the primary distillation of oil. The middle distillate fraction contains a significant amount of higher n-alkanes.

In [9], researchers consider the process of reducing the sulfur content in the middle distillate fraction due to the hydrogen-containing gas. It is well known that one of the quality indicators of winter diesel fuel is sulfur content. This indicator depends on the sulfur content of the starting components, after compounding of which winter diesel fuel is obtained. The base component for compounding is just the denormalizate, which is obtained after dewaxing of the corresponding components.

In [10], researchers analyze the influence of technological parameters on the properties of the cooling stream and, thereby, on the yield of denormalizate after dewaxing. Higher n-alkanes (C_{24-36} , for example) crystallize with decreasing temperature and bind the liquid phase. Figuratively speaking, winter diesel fuel with a high content of higher n-alkanes will thicken at low temperatures, making the diesel engine impossible to operate. Therefore, the higher n-alkanes are removed at the dewaxing stage. One way is to lower the temperature of the raw material. That is, in producing winter diesel fuel we expose the feedstock to low temperatures in order to remove the highest n-alkanes as much as possible. If we consider the catalytic dewaxing processes, then the use of synthetic zeolite enriched with rare earth elements (La, Ce, etc.) is widespread.

In [11], researchers use quantum mechanical equations to assess the thermodynamics of desulfurization processes, which ensures high reliability of the theoretical approach.

In [12], researchers propose for consideration a nontrivial mathematical model of catalytic dewaxing.

In [13], researchers consider the question of how the hydrocarbon composition of the feedstock affects the quality indicators of the obtained winter diesel fuel.

In [14], researchers presented a mathematical model for the catalytic isomerization of light naphtha. For light naphtha, the initial boiling point is 30 °C, and the end boiling point is 70 °C.

In [15], researchers analyze the process of reducing the activity of the catalyst due to the effect of coke and heavy metals.

In [16], researchers apply multi-criteria optimization. They use winter diesel quality indicators as criteria. Each of the compounding components has its own quality limitations.

The given literature review is not exhaustive, but it gives an idea of the main approaches to improving the low-temperature properties of WDF:

1. catalytic dewaxing;
2. dewaxing by lowering the temperature of the raw material;
3. reduction of the sulfur content in the feedstock.

Also worth mentioning is a method such as catalytic isomerization (quite expensive due to the use of platinoids as catalysts).

Basic research methods: retrospective analysis of mathematical models for obtaining WDF, synthesis, comparison, methods of mathematical programming.

3 Results

Research hypothesis: combining dewaxing modes will increase the yield of the normalizer and, subsequently, the yield of winter diesel fuel.

Basic model assumptions:

The first stage of obtaining WDF is the dewaxing of a mixture of a hydrotreated diesel fraction 200–320°C (hereinafter referred to as DF_1 , or x_1), a hydrogen-containing gas

(hereinafter referred to as HCG, or x_2), and a hydro treated WDF (hereinafter referred to as HTWDFd, or x_3). The process is calculated on the target raw materials. The target raw material is a mixture of DF1 and HTWDF. HCG is a working medium in which paraffins are released on zeolites. The product yield depends only on the target raw material. In this study, we will consider the operation of the dewaxing unit in four modes.

After dewaxing in each mode, we get:

1. denormalize (x_{4i});
2. desorbate (x_{5i});
3. losses (x_{6i});
4. a mixture of hydrocarbon gas (hereinafter referred to as HG) with HCG (x_{7i}).

Here index i takes values from 1 to 4, which corresponds to one of the operating modes of the dewaxing unit.

For each mode, each type of product (x_{4i} , x_{5i} , x_{6i} , x_{7i}), respectively, has its own selection coefficients (k_{4i} , k_{5i} , k_{6i} , k_{7i}). In each mode, the unit processes a certain share of the target raw material. We set these shares, respectively, as d_1 , d_2 , d_3 , d_4 .

The second index indicates in which mode the unit is operating. Then, for each mode, you can write down the corresponding equations.

The first operating mode of the dewaxing unit:

$$d_1(x_1 + x_3) + \alpha_{21}d_1(x_1 + x_3) = x_{41} + x_{51} + x_{61} + x_{71} \quad (1)$$

$$x_{41} - k_{41}d_1(x_1 + x_3) = 0 \quad (2)$$

$$x_{51} - k_{51}d_1(x_1 + x_3) = 0 \quad (3)$$

$$x_{61} - k_{61}d_1(x_1 + x_3) = 0 \quad (4)$$

$$x_{71} - k_{71}d_1(x_1 + x_3) = 0 \quad (5)$$

$$k_{41} + k_{51} + k_{61} + k_{71} - 1 - \alpha_{21} = 0 \quad (6)$$

The second operating mode of the dewaxing unit:

$$d_2(x_1 + x_3) + \alpha_{22}d_2(x_1 + x_3) = x_{42} + x_{52} + x_{62} + x_{72} \quad (1')$$

$$x_{42} - k_{42}d_2(x_1 + x_3) = 0 \quad (2')$$

$$x_{52} - k_{52}d_2(x_1 + x_3) = 0 \quad (3')$$

$$x_{62} - k_{62}d_2(x_1 + x_3) = 0 \quad (4')$$

$$x_{72} - k_{72}d_2(x_1 + x_3) = 0 \quad (5')$$

$$k_{42} + k_{52} + k_{62} + k_{72} - 1 - \alpha_{22} = 0 \quad (6')$$

The third operating mode of the dewaxing unit:

$$d_3(x_1 + x_3) + \alpha_{23}d_3(x_1 + x_3) = x_{43} + x_{53} + x_{63} + x_{73} \quad (1'')$$

$$x_{43} - k_{43}d_3(x_1 + x_3) = 0 \quad (2'')$$

$$x_{53} - k_{53}d_3(x_1 + x_3) = 0 \quad (3'')$$

$$x_{63} - k_{63}d_3(x_1 + x_3) = 0 \quad (4'')$$

$$x_{73} - k_{73}d_3(x_1 + x_3) = 0 \quad (5'')$$

$$k_{43} + k_{53} + k_{63} + k_{73} - 1 - \alpha_{23} = 0 \quad (6'')$$

The fourth operating mode of the installation:

$$d_4(x_1 + x_3) + \alpha_{24}d_4(x_1 + x_3) = x_{44} + x_{54} + x_{64} + x_{74} \tag{1'''}$$
$$x_{44} - k_{44}d_4(x_1 + x_3) = 0 \tag{2'''}$$
$$x_{54} - k_{54}d_4(x_1 + x_3) = 0 \tag{3'''}$$
$$x_{64} - k_{64}d_4(x_1 + x_3) = 0 \tag{4'''}$$
$$x_{74} - k_{74}d_4(x_1 + x_3) = 0 \tag{5'''}$$

For the entire dewaxing unit, it is also true:

$$x_1 + x_3 \leq A \tag{7}$$
$$x_1 + x_3 \leq B \tag{8}$$

where:

- A, B are the boundaries of the capacity of the dewaxing unit;
- (1) is the mass balance equation for the 1st mode;
- (2) is the equation of the output of the denormalize for the 1st mode;
- (3) is the equation of the desorbate yield for the 1st mode;
- (4) is the equation of the loss output for the 1st mode;
- (5) is the equation of the yield of the mixture of HG and HCG for the 1st mode;
- (6) shows that the sum of the selection coefficients exceeds 1 exactly by the HCG coefficient;
- (7) and (8) are the limitations on the capacity of the unit.
- By analogy with the equations for the first mode, equations for the other three modes are compiled.

For the first stage, there is no need to set the ratio of the components DF1 and HTWDFd, since they (within the framework of this process) have similar properties and can be mixed in any proportion.

II. The second stage of obtaining WDF is compounding of denormalize (hereinafter referred to as x_4), diesel fraction 150–310°C (hereinafter referred to as DF2, or x_8), and hydro treated WDF (x_9). We draw up a system of constraints on the quality of WDF, write down the objective function (hereinafter referred to as OF) and maximize profit.

Denormalize (x_4) obtained at the first stage participates in the second stage, compounding. Moreover, the number of DF2 (x_8) and HTWDFc (x_9) can be specified as part of the amount of denormalize (x_4).

As a result of the second stage, it is required to reach the specified quality of the WDF. Quality indicators are represented in table 1.

Table 1. Quality indicators of components for compounding and WDF.

No.	Substance	ρ , kg/m3	s, ppm	t flash, °C
1	Denormalize (x_4)	$\rho_4 = 832.4$	$s_4 = 2$	$t_4 = 72$
2	HTWDFk (x_9)	$\rho_9 = 786.4$	$s_9 = 10$	$t_9 = 34.5$
3	DF2 (x_8)	$\rho_8 = 798$	$s_8 = 1.3$	$t_8 = 41$
4	WDF (x_{10})	$\rho_{\min} = 800$ $\rho_{\max} = 840$	$s_{10} = 10$	$t_{10} = 40$

$$x_4 + x_8 + x_9 = x_{10} \tag{9}$$

$$x_4 = x_{41} + x_{42} + x_{43} + x_{44} \tag{10}$$

$$x_8 = \beta_1 x_4 \tag{11}$$

$$x_9 = \beta_2 x_4 \tag{12}$$

$$s_{10}x_{10} - s_4x_4 - s_8x_8 - s_9x_9 \leq 0 \quad (13)$$

$$x_{10}t_{10} = x_4t_4 + x_8t_8 + x_9t_9 \quad (14)$$

$$x_{10}\rho_{min} \leq x_4\rho_4 + x_8\rho_8 + x_9\rho_9 \quad (15)$$

$$x_{10}\rho_{max} \leq x_4\rho_4 + x_8\rho_8 + x_9\rho_9 \quad (16)$$

where:

(9) is the weight balance;

(10) is the total volume of the denormalize as the sum of the quantities obtained in each mode;

(11) specifies DF2 as a share of the denormalize;

(12) specifies HTWDFc as a share of the denormalize;

(13) is the condition for sulfur content of WDF;

(14) is the balance by conventional ton-degrees;

(15) is the condition for ρ_{min} by conventional ton-density;

(16) is the condition for ρ_{max} by conventional ton-density.

From (12, 13, 14):

$$x_{10} - x_4(1 + \beta_1 + \beta_2) = 0 \quad (17)$$

Taking into account (11, 12), we rewrite (13, 14, 15, 16) in the form:

$$s_{10}x_{10} - x_4(s_4 + s_8\beta_1 + s_9\beta_2) \leq 0 \quad (13')$$

$$x_{10}t_{10} - x_4(t_4 + t_8\beta_1 + t_9\beta_2) = 0 \quad (14')$$

$$x_{10}\rho_{min} - x_4(\rho_4 + \rho_8\beta_1 + \rho_9\beta_2) \leq 0 \quad (15')$$

$$x_{10}\rho_{max} - x_4(\rho_4 + \rho_8\beta_1 + \rho_9\beta_2) \geq 0 \quad (16')$$

The objective function can be written as

$$OF = \rho_{10}x_{10} + \rho_5x_5 + \rho_7x_7 - c_1x_1 - c_3x_3 - c_8x_8 - c_9x_9 \rightarrow \max \quad (18)$$

where:

$\rho_{10}, \rho_5, \rho_7$ are the prices of WDF, desorbate and hydrocarbon gas, rubles/ton;

c_1, c_3, c_8, c_9 are the costs per ton of the corresponding component.

Then the mathematical model for obtaining WDF with a combination of dewaxing modes is as follows:

$$OF = \rho_{10}x_{10} + \rho_5x_5 + \rho_7x_7 - c_1x_1 - c_3x_3 - c_8\beta_1x_4 - c_9\beta_2x_4 \rightarrow \max \quad (18')$$

$$x_4 = (x_1 + x_3) \sum_{i=1}^4 k_{4i}d_i \quad (19)$$

$$x_5 = (x_1 + x_3) \sum_{i=1}^4 k_{5i}d_i \quad (20)$$

$$x_7 = (x_1 + x_3) \sum_{i=1}^4 k_{7i}d_i \quad (20)$$

$$k_{41} + k_{51} + k_{61} + k_{71} - 1 - \alpha_{21} = 0 \quad (6)$$

$$k_{42} + k_{52} + k_{62} + k_{72} - 1 - \alpha_{22} = 0 \quad (6')$$

$$k_{43} + k_{53} + k_{63} + k_{73} - 1 - \alpha_{23} = 0 \quad (6'')$$

$$k_{44} + k_{54} + k_{64} + k_{74} - 1 - \alpha_{24} = 0 \quad (6''')$$

$$x_{10} - x_4(1 + \beta_1 + \beta_2) = 0 \quad (17)$$

$$s_{10}x_{10} - x_4(s_4 + s_8\beta_1 + s_9\beta_2) \leq 0 \quad (13')$$

$$x_{10}t_{10} - x_4(t_4 + t_8\beta_1 + t_9\beta_2) = 0 \quad (14')$$

$$x_{10}\rho_{min} - x_4(\rho_4 + \rho_8\beta_1 + \rho_9\beta_2) \leq 0 \quad (15')$$

$$x_{10}\rho_{max} - x_4(\rho_4 + \rho_8\beta_1 + \rho_9\beta_2) \geq 0 \quad (16')$$

$$x_1 + x_3 \leq A \quad (7)$$

$$x_1 + x_3 \leq B \quad (8)$$

$$\sum_{i=1}^4 d_i = 1 \quad (22)$$

It seems possible to use the corresponding kind of the simplex method to solve this problem.

Let's take into account the logistic aspect. Fig. 1 schematically shows the storage of WDF at a refinery.

Fig. 1. The storage of WDF at a refinery.

The resulting WDF, relatively speaking, is stored in a tank with a capacity of Q . The amount of WDF should not be less than the demand for WDF for winter period equal to D . We will restrict ourselves to the location of the consumer, St. Petersburg and the Leningrad Region. Winter time there is 5.5 months and lasts from November 1 to April 15.

The amount of WDF in the tank can be described by the differential equation

$$\frac{dx_{10}}{dt} = -q_{10}x_{10} \quad (23)$$

Where

$$q_{10} = \frac{r_{10}}{Q} \quad (24)$$

r_{10} is the rate of WDF entering the tank (technological indicator, can be determined in the compounding process), tons/sec.

Accordingly,

$$x_{10}(t = 0); x_{10}(t = T) \geq D \quad (25)$$

Having supplemented the original MMWDFd with conditions (23), (24), (25), we will introduce the dynamics and the requirement of demand correspondence into the mathematical model of obtaining WDF for the case of a combination of the dewaxing modes.

4 Discussion

A mathematical model of a combination of dewaxing modes is obtained. The main hypothesis is that the operating time of the dewaxing unit in the i -th mode can be set as a fraction of one. In other words, during the operation in the i -th mode, the corresponding share of the feedstock is processed. The sum of the shares, respectively, is equal to one. The operation of the dewaxing unit in the i -th mode can be described by linear dependencies. Next, we aggregate all our dependencies across all four (for our case) modes. In general, the owner of the dewaxing unit (oil refinery) can set the number of modes. Then we compose an objective function aimed at maximizing profits. It remains to solve the resulting linear programming problem. Solution methods are known.

The developed mathematical model continues the line outlined in a number of articles devoted to the digitalization of the processes of obtaining and using energy resources, as well as the problems associated with the development of regions of the Arctic and the Great Northern Sea Route [17–21].

5 Conclusions

In this study, the authors have obtained the following outcomes. A mathematical model has been built for digitalizing oil-refining processes in winter diesel fuel production, taking into account the combination of 4 dewaxing modes.

A method for solving the mathematical model for obtaining winter diesel fuel is proposed. It is a kind of simplex method.

The initial mathematical model for obtaining winter diesel fuel, taking into account the combination of the dewaxing modes, is supplemented with the logistic aspect. For this, an example of consumer location in St. Petersburg and the Leningrad Region is considered, which made it possible to introduce dynamics and compliance with demand requirements into the mathematical model.

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