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Procedia Chemistry 10 (2014) 289 – 296

Procedia Chemistry

XV International Scientific Conference “Chemistry and Chemical Engineering in XXI century” dedicated to Professor L.P. Kulyov

Complex system for gasoline blending maintenance

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Abstract

The main aim of the study is to increase the efficiency of gasoline blending process using developed complex modeling system, it provides counting feedstock changes in the refinery, influencing detonation characteristics of trade gasoline. Final products of modeling system are precise and gasoline blending recipes are economically optimal. The relevance of the study is caused by the need to increase production volumes of trade gasoline in refineries that meet gasoline quality standards. Mathematical modeling and application of automatic computer systems are most relevant solutions for optimization of technologically difficult stages of oil production. The study considers the modeling approach to the blending process from the position of non-additivity of gasoline octane numbers. Practical results: The module of gasoline detonation characteristics developed in Borland «Delphi 7» workspace in conjunction with the module of chromatographic data analysis «Unichrom» and optimal recipes development module are combined in the universal complex system for gasoline blending process maintenance. The system allows taking into account feedstock composition changes on purpose to vary the recipes of trade gasoline blending. The developed complex system analyzes refinery conditions and recommends the feedstock supply in the process and allows getting essential economic benefit for the refineries by reducing the quality reserve of trade products.

Peer-review under responsibility of Tomsk Polytechnic University

Keywords: Blending; octane number; modeling; non-additivity; chromatographic data analysis; gasoline recipes.

1. Introduction

Continious functioning of the modern refinery is impossible without application of automatic computer systems. They provide continuous monitoring and control of technological processes, as well as collecting, storing and

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Peer-review under responsibility of Tomsk Polytechnic University
doi:10.1016/j.proche.2014.10.049

processing of large amounts of information. Refineries are searching for most effective modeling and control systems that could provide the optimal management of processes in order to increase their energy and resource efficiency.

Computer systems accurately reproducing chemical and technological processes by virtual models are especially relevant in modern refining industry.

In this way, models for reforming, alkylation, and isomerization processes were developed and implemented in the technological scheme. They combine the knowledge of thermodynamics, kinetics, chemical nature of reactions, and also influence on technological parameters and specific features of production units. It provides monitoring and long-term forecasting of target secondary refining processes components production.

Gasoline is one of the most desired products of oil refinery all over the world; production of gasoline is an actual and perspective technology. In spite of rise in popularity of biodiesel and other alternative fuels increase in trade gasoline production volumes is obvious in most countries.

Blending is an important technological process providing the production of high-octane gasoline by mixing straight-run oil fractions with secondary refining processes components and special additives. This process as the final stage of gasoline production determines its qualitative and quantitative characteristics. In the view of tightening norms for gasoline quality and optimal management standpoint, optimization of the blending process is a actual goal for refinery.

In the same time, this process is one of the most difficult technologies for optimization. This is primarily due to a large number of different components involved in the blending process, the composition and physical properties of which vary considerably.

Thus, the first difficulty is the impossibility of a universal recipe for any brand of gasoline development. It does not seem to be possible even within the same refinery due to permanent changes of feedstock hydrocarbon composition.

Production regime, presence of definite volumes of feedstock components forces to revise existing recipes in real time in order to meet gasoline quality standards. It makes continuous planning and prediction of technological processes an integral part of refinery.

The most unpredictable factor hindering the blending process is the non-additive nature of mixture octane numbers. As the most important detonation characteristic of gasoline, it is not subjected to the law of additivity. It is caused by intermolecular interactions of gasoline mixture leading to changes in molecular configurations and, as a result, it eventually influences mixture final octane number.

Therefore, deep knowledge of physic-chemical basis of the blending process optimization is required. Application of modeling systems based on adequate mathematical models is an effective method for solving these multi-factorial and multi-criteria optimization tasks. It provides calculating the most appropriate and precise blending recipes and finally results in the essential economic benefit and an increase in the efficiency of the blending stage in general.

Considering modern software market of modeling systems for refineries, such commercial packages as Aspen Process Industry Modeling System (Aspen PIMS) of Aspen Technology Inc. and Blend Optimization and Supervisory System (BOSS) of Invensys plc. should be noted. They provide automatic calculations of economically optimal gasoline recipes according to price analysis and refinery conditions. Moreover, it contains an extensive database for thousands of substances, processes and devices and gives the possibility of economic planning and processes management in general[1]. However, despite all advantages of these programs, calculation could not take into account intermolecular interaction of gasoline components, so it leads to significant errors complicating the control of blending process in general. One of existing solutions is using correlation coefficients in the blending process. For every volume of trade product they differ from each other due to changes of hydrocarbon composition of feedstock. As a result, this method is neither universal nor absolutely accurate.

2. Ways of gasoline blending optimization

Increasing the energy and resource efficiency of refinery is a highly relevant direction of scientific activity. Therefore, there are a lot of researches related to this topic. Firstly, it means octane number and production volumes increase and gasoline production costs reduction. To achieve the product with specified quality, it is necessary to decrease the aromatics, sulfur and benzene content. These measures are directed to optimize technological and catalysts efficiency of both modeling and control systems application.

The authors of[2] consider reduction of the benzene content in reformates reached with the combination of two catalysts, already tested in the laboratory. It provides effective benzene conversion to methylcyclopentane and normal paraffins C_5-C_7 isomerization reactions.

It provides a perspective way of the high-octane alkylate component of gasoline production in domestic refineries.

In the paper[3] the blending process for light products in the Arak Refinery is described with linear planning technique using Lingo software. As a result, the authors claim that profit of refinery has to be maximized.

The case study[4] was conducted regarding the physical and chemical properties of key gasoline oxygenates, such as methyl tertiary butyl ether (MTBE), tertiary amyl methyl ether (TAME) and other blending components. It was shown that oxygenates are an effective way to preserve octane number in domestic refineries.

Thus, using high-octane components and improving the production technology are an effective way to optimize the blending process. However, as it was shown above, using of modeling systems, based on mathematical models is a perspective instrument to achieve quality monitoring, forecasting and resource efficient management of blending process.

In this way, optimization of blending process requires precise analytic dependences for determination of octane rating. Currently, it is generally accepted to use models describing mechanisms of hydrocarbons and anti-knock additives influence and gasoline properties used to calculate precise mixture octane number. The most common ones are hydrocarbon composition, structure, density, absorption spectrum, the permittivity, the degree of compression and the degree of refractive index, etc.

These methods are usually divided into the following categories:

- Detonation resistance of gasoline is connected with its physic-chemical properties.
- Detonation resistance of gasoline depends on hydrocarbon components composition.
- Reactivity of components is counted to calculate detonation resistance of mixture.

The first papers about this subject appeared in the 1960s. They described linear dependences and formulas based on component formulation and group hydrocarbon gasoline composition. In the further papers as[5], correlation between octane number and physic-chemical properties of gasoline quality were analyzed. It was concluded that significant correlation between octane number and vapor pressure, density and fractional composition commonly occur in practice.

The authors of papers[6,7] offered a method of counting quality characteristics of oil feedstock involved into blending. It could be applied for solving the problem of optimal blending recipes searching. It was suggested that all basic physic-chemical properties (as density, octane number, fractional composition and sulfur content) are additive in the mass or volume with enough accuracy for practical purposes.

In the papers[5,8] the main properties of gasoline, measured in refinery, were researched. Analysis of couple correlation showed significant interdependence between octane number, saturated vapor pressure, density and fractional composition properties. The authors gave formulas for calculations of all parameters in form of linear regression equations. The main drawback of these equations is necessity of precise values of the coefficients for every definite refinery unit. When feedstock composition significantly changes, these coefficients have to be recalculated.

The author[9] investigated the dependence of physical properties of hydrocarbons: the molecular weight, boiling point and density on the detonation of gasoline.

Efficient modeling systems with predictive abilities could be created on the basis of advanced computer technologies. One of the first models for blending process described in[10] is the “ideal” model, where gasoline components have been mixed by linear model according to their fractional volumes. The other method based on application of artificial neural networks for predicting octane number for gasoline blends is considered in[11,12].

3. Complex system for gasoline blending maintenance

A new approach for gasoline blending process calculation was suggested by the department of Chemical Technology of Fuel and Chemical cybernetics of National Research Tomsk Polytechnic University. The authors of the theory[13] described the nature of blending analysis of existing octane numbers deviations from the law of additivity. It was revealed that differences in the properties of individual components in a free condition and in mixtures with other hydrocarbons take place in every hydrocarbon stream.

Precise analysis of intermolecular interactions makes it possible to consider the change of content of involved feedstock, technological parameters and specific features of production units[14-17]. Values of *Bi* coefficients considering the non-additivity of octane numbers for certain substances are given in Table. 1.

Table 1. Values of *Bi* coefficients for certain substances

№	Component	*Bi*	№	Component	*Bi*	№	Component	*Bi*
1	n-pentane	0.16	6	2,2,3-trimethylbutane	0.07	11	toluene	0.6
2	n-heptane	0.1	7	2,4-dimethylhexane	0.26	12	xylols	-0.57
3	i-butane	0.17	8	cyclopentane	0	13	butene-1	1.28
4	2-methylpentane	0.2	9	methylcyclohexane	0.22	14	pentene-2	1.25
5	2,3-dimethylbutane	0.16	10	benzene	0.98	15	heptene-3	0.8

The dependence of hydrocarbon content on the octane number deviations is revealed on the basis of experimental data and shown in[13] as a set of equations. These equations are formed on the basis of calculation module for blending process. Its main function is providing calculations for required detonation characteristics of gasoline:

- Octane number of hydrocarbon stream involved into the blending process taking into account their non-additivity by the research and motor method;
- Aromatics, olefins hydrocarbons and benzene percentage;
- Saturated vapor pressure (SVP), density and viscosity of gasoline.

The module is developed in Borland «Delphi 7» workspace combining a user-friendly interface and stable functioning. This module is combined with the module of input data formation «Unichrom» and optimal recipes development module in the universal complex system for gasoline blending process maintenance. The scheme of the system is shown in Fig. 1.

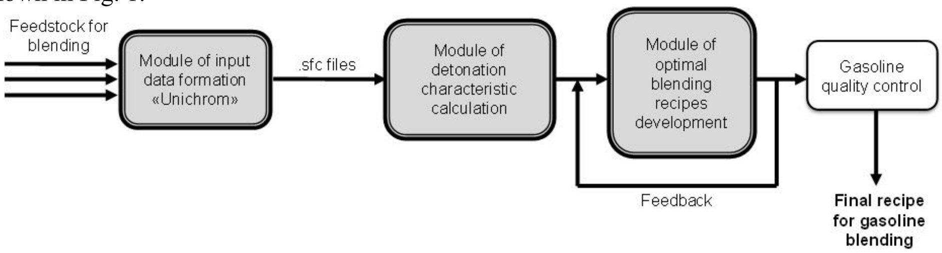

Fig. 1. The scheme of complex system for gasoline blending maintenance

The module of optimal recipes development is a program implemented on the basis of logical algorithm. It provides an effective involvement of feedstock steams, starting from reformate, as represented in the greatest volumes in the refinery, then catalytic cracking gasoline, finishing with high-qualitative and the most expensive components such as isomerizate, alkylates and anti-knock additives. Within this technology, all gasoline quality parameters are strictly controlled. It is ensured with precise calculations of octane number, SVP and aromatics, olefins hydrocarbons and benzene percentage for every gasoline recipe. Hydrocarbon composition of feedstock is taken from the module of input data formation.

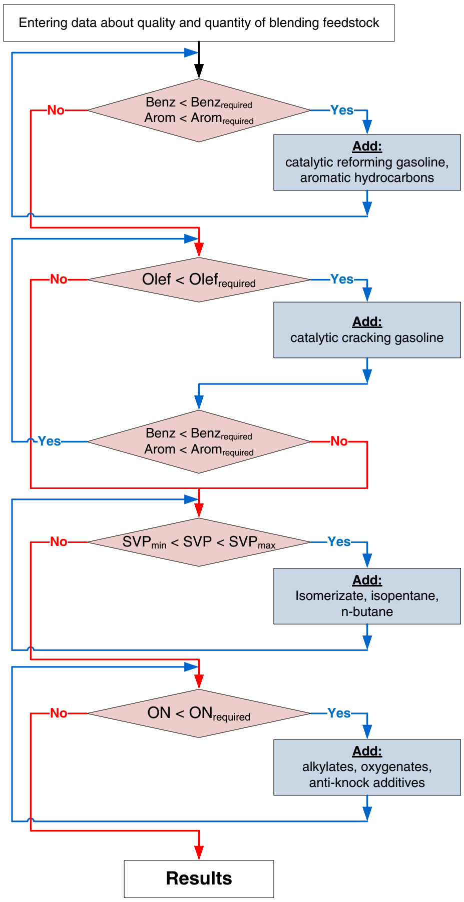

Fig. 2. The logical algorithm of optimal recipes development module

For this figure:

Benz, Arom, Olef – benzene, aromatics and olefins content in gasoline, respectively;

$Benz_{required}$, $Arom_{required}$, $Olef_{required}$ – required benzene, aromatics and olefins content in gasoline, according to environmental standards;

SVP – saturated vapor pressure of gasoline; $SVP_{required}$ – required saturated vapor pressure of gasoline, according to environmental standards;

ON – octane number of gasoline; $ON_{required}$ – required octane number of gasoline, according to environmental standards.

4. Developing recipes for gasoline blending

The main goal of work is to develop recipes for gasoline blending with the lowest cost of components, involvement of all volumes of available feedstock. At the same time, complex system provides all necessary calculations to produce gasoline according to modern quality standards.

Feedstock flow rate is the most important automatically controlled technological parameter that largely influences the production of gasoline. The tables below show how different total reformate flow rate influences the recipe and quality of 3 brands of trade gasoline: Regular-92, Premium-95 and Super-98.

Table 2. Influence of the reformate flow rate on the flow rate of components for the production of gasoline

Feedstock flows	Flow rate, tons/hour		
Reformate	80	90	100
Isomerizate	35	30	30
Catalytic cracking gasoline	100	100	90
Alkylate	35	35	40
Isopentane	35	35	35
MTBE	15	10	5
TOTAL, tons/hour	300	300	300

Table 3. Gasoline recipes and quality characteristics of reformate flow rate of 80 tons/hour

Feedstock flows	Euro-3 quality standard and above			Flow rate, tons/hour
	Regular-92	Premium-95	Super-98	
Reformate	26	28	26	80
Isomerizate	10	10	15	35
Catalytic cracking gasoline	47	38	15	100
Alkylate	7	10	18	35
Isopentane	10	9	16	35
MTBE	–	5	10	15
TOTAL, tons/hour	***100***	***100***	***100***	***300***
RON	**92.5**	**95.1**	**98.5**	
Benzene, % wt.	0.81	0.8	0.62	
Aromatics, % wt.	32.35	32.07	24.83	
Olefins, % wt.	7.77	6.37	2.51	
SVP, kPa	54.68	52.96	64.8	

Table 4. Gasoline recipes and quality characteristics of reformate flow rate of 90 tons/hour

Feedstock flows	Euro-3 quality standard and above			Flow rate, tons/hour
	Regular-92	Premium-95	Super-98	
Reformate	26	31	33	90
Isomerizate	14	6	10	30
Catalytic cracking gasoline	47	38	15	100
Alkylate	3	12	20	35
Isopentane	10	9	16	35
MTBE	–	4	6	10
TOTAL, tons/hour	***100***	***100***	***100***	***300***
RON	**92.4**	**95.1**	**98.0**	
Benzene, % wt.	0.82	0.86	0.76	
Aromatics, % wt.	32.66	34.51	30.51	
Olefins, % wt.	7.85	6.37	2.51	

SVP, kPa	58.97	48.07	57.85	

Table 5. Gasoline recipes and quality characteristics of reformate flow rate of 100 tons/hour

Feedstock flows	Euro-3 quality standard and above			Flow rate, tons/hour
	Regular-92	Premium-95	Super-98	
Reformate	28	33	39	100
Isomerizate	13	11	6	30
Catalytic cracking gasoline	47	31	12	90
Alkylate	2	14	24	40
Isopentane	10	9	16	35
MTBE	–	2	3	5
TOTAL, tons/hour	***100***	***100***	***100***	***300***
RON	**92.5**	**95.3**	**98.0**	
Benzene, % wt.	0.86	0.86	0.86	
Aromatics, % wt.	34.28	34.43	34.64	
Olefins, % wt.	7.85	5.19	2.03	
SVP, kPa	57.45	52.37	52.04	

It can be concluded that the increase in flow rate of reformate from 80 tons/hour to 90 tons/hour allows reducing flow rate of isomerizate by 5 tons/hour and flow rate of MTBE by 5 tons/hour.

At the same time, detonation characteristics and final recipes vary significantly; for example, flow rate of expensive anti-knock additive MTBE is reduced while flow rate of reformate increases from 80 tons/hour to 90 tons/hour, so it provides economical benefit for refinery.

Another technological option is to increase flow rate of reformate from 90 tons/hour to 100 tons/hour. As a result, it affects reducing the MTBE flow rate for another 5 tons/hour, from 10 to 5 tons/hour. However, it requires the increase in alkylate flow rate to 40 tons/hour.

The decision is taken according to current production and economic conditions, presence of components in the refinery and their price.

All calculations could be processed by the modeling system in real-time mode based on the chromatography data results for final decision of gasoline recipe.

5. Conclusions

The developed complex system for gasoline blending process maintenance allows precise calculation of streams hydrocarbon composition and detonation characteristics of gasoline.

It alters flow rates and hydrocarbon composition of feedstock and develops economically optimal blending recipes of trade gasoline. The complex system analyzes refinery conditions and recommends optimal feedstock supply.

Precision of the developed recipes saves expensive components and provides essential economic benefit for the refineries by improving the quality of trade products while reducing gasoline production costs. In general it reflects the idea of continuous monitoring and quality control of the blending process in the refinery.

Acknowledgements

This work was supported by the grant of the President of the Russian Federation for state support of leading scientific schools NSH-422.2014.8.

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