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COMPUTER SIMULATOR FOR STUDENT TRAINING TO EFFECTIVE EXPLOITATION THE CATALYTIC CRACKING UNIT

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Abstract

Entering the electronic educational resources into the structure of academic studies is important stage to implementation of competency-based approach at preparation of technologists. This paper describes a creation of the computer simulator for student training to effective exploitation the catalytic cracking unit. Computer simulator was built on the basis of mathematical model of catalytic cracking and included as the e-learning tool. Mathematical model was development on the basis of thermodynamically and kinetic approach. The mathematical model of the process was developed and implemented using Delphi 7 software. The calculation result had shown a high adequacy that's allowed to use a mathematical model as a computer simulator for training to effective exploitation the catalytic cracking unit. Developed computer simulator was entered to the cycle of laboratory works. Pedagogical design of the laboratory work was performed using Adobe Dreamweaver CS 5.5 and iSpring Suite 7 software. Computer simulator "Catalytic Cracking" is designed to educate the efficient exploitation of industrial catalytic cracking unit and can be used on Higher Education.

Keywords: thermodynamic; kinetic; catalytic cracking; computer simulator; preparation of technologists; competence-based approach.

1. Introduction

During operation of industrial oil installations, it is important to consider the multifold factors that equally influence composition, quantity, and quality of the main products [1-8]. The optimization of multicomponent petroleum refining processes can be solved by the development of adequate mathematical model based on physical and chemical regularities of process reactions [9-18].

Since the High Education has important role at preparation of technologists for oil refining and such mathematical model can be used for training of students to operate of industrial unit in education process. At the present time computers of educational systems aimed at achieving a high level of assimilation of information are being actively implemented in the educational process [19].

This paper describes a creation of the computer simulator for student training to effective exploitation the catalytic cracking unit. The purpose of this work is developing and program realization of computer simulator on the basis of mathematical model of catalytic cracking for technologists preparation to operate at catalytic cracking unit.

The relevance of this paper is defined by an introduction of developed mathematical model of advanced petroleum process in the educational process in order to improve the assimilation of information about technological features and pattern of existing facilities refining.

2. Experimental

2.1. Formalization of the hydrocarbon conversion scheme of catalytic cracking

The catalytic cracking process is used for the production of gasoline, diesel fractions, and

gas via catalytic cracking of vacuum distillate hydrocarbons or a mixture of residues of secondary processes (350–570°C fractions).

The mathematical model of the catalytic cracking was developed on the basis of a formalized hydrocarbon conversion scheme and is leading in the basis of the computer simulator "Catalytic Cracking".

Data concerning quantitative and qualitative groups composition of catalytic cracking feedstock and individual composition of gasoline fraction is required for the development of the mathematical model of catalytic cracking. Laboratory investigations were performed in the Tomsk Polytechnic University [20].

According to the results of laboratory investigation had been compiled list reactions of the catalytic cracking. The thermodynamic parameters of the catalytic cracking reactions were determined using Density Functional Theory. The DFT method was chosen as the main method of calculation. The B3LYP (Becke's density functional theory (B3) model using Lee-Young-Parr (LYP) electron correlation) with basis 3-21G were used as theoretical approximation [21].

Models of the substances involved in the reactions have been built using GaussView software (fig. 1).

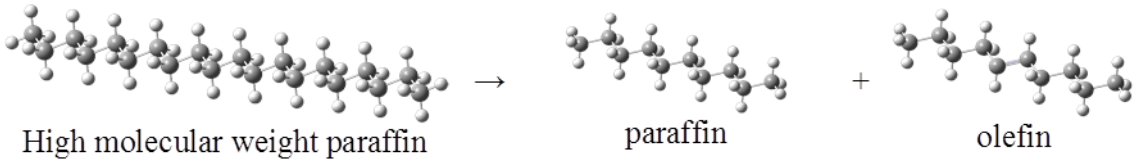

Figure 1. Example of cracking reaction (GaussView software)

The average results of thermodynamic parameters of catalytic cracking reactions are listed in tab. 1.

Table 1. Averaged results of thermodynamic parameters of catalytic cracking reactions (T=777 K, Pressure=1.08 MPa)

Reaction	ΔG, kJ/mole	ΔH, kJ/mole
Conversion of feedstock (primary reactions)		
Cracking of paraffins C_{13}–C_{40}	-74.32	69.5
Cracking of paraffins C_{13}–C_{40} to isoparaffins	-76.82	73.75
Dealkylation of naphthenes	-120.4	118.14
Dealkylation of aromatics	-91.68	128.2
Cracking of polynaphthenes	-69.7	221.3
Secondary reactions		
Cracking of paraffins C_5–C_{11+}	-62.27	73.6
Cracking of isoparaffins C_5–C_{11+}	-63.21	65.18
Isomerization of paraffins C_5–C_{11+}	-2.34	-1.78
Cracking of olefins C_5–C_{11+}	-28.28	92.72
Cyclization of olefins	-7.5	-53.8
Hydrogen transfer	-111.76	74.25
Coke formation (polycondensation)	-594.2	-103.73

According to calculation results the primary catalytic cracking reactions are characterized a high thermodynamic of the probability with endothermic effect. The Gibbs energy change lie in the interval ΔG = −69.7 ÷ −124.63 kJ/mol and thermal effect lie in the interval ΔH = 69.5 ÷ 221.3 kJ/mol for the above reaction. The most thermodynamically probable from secondary reaction is hydrogen transfer (ΔG = −111.76 kJ/mol) and polycondensation (ΔG = −594.2 kJ/mol).

Formalized hydrocarbon conversion scheme was compiled based on thermodynamic analysis, experimental data from industrial unit and laboratory investigation of catalytic cracking raw materials and product performed in Tomsk Polytechnic University (fig. 2).

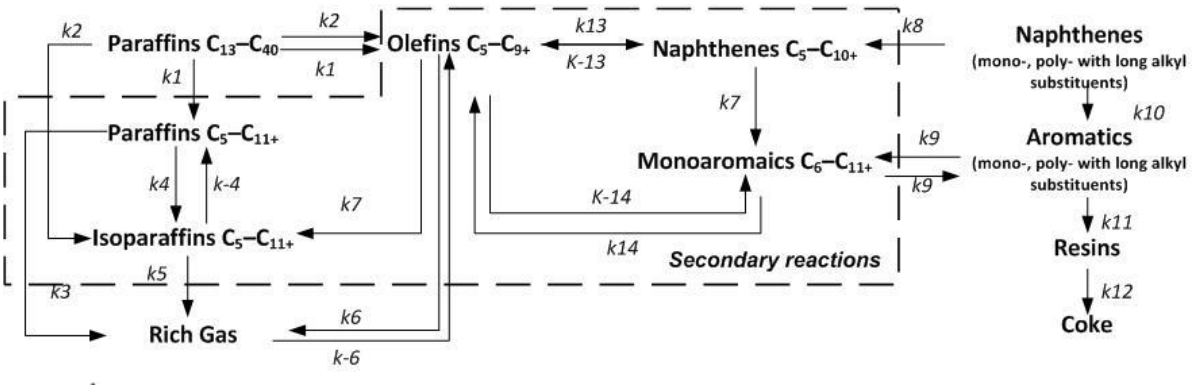

Figure 2. Formalized hydrocarbon conversion scheme of catalytic cracking

2.2. Development of computer simulator of the catalytic cracking unit

The kinetic model of the catalytic cracking is developed on the basis of the formalized hydrocarbon conversion scheme. The kinetic model of the catalytic cracking describes the change in concentration of the reactants depending on contact time with the initial conditions: $\tau = 0$, $C_i = C_{i0}$, where i is the corresponding hydrocarbon. The expressions for the reaction rate constants are written according to the law of mass action (tab. 2).

Table 2. Expressions for rates of reactions in catalytic cracking

Component	Reaction rate expression	
	direct reaction	reverse reaction
Cracking of paraffins $C_{13}–C_{40}$	$W_1=k_1C_{paraffinsHMW}$	-
Cracking of paraffins $C_{13}–C_{40}$	$W_2=k_2C_{paraffinsMMW}$	-
Cracking of paraffins $C_5–C_{11+}$	$W_3=k_3C_{paraffinsMMW}$	-
Isomerization of paraffins $C_5–C_{11+}$	$W_4=k_4C_{paraffinsMMW}$	$W_{-4}=k_{-4}C_{isoparaffins}$
Cracking of isoparaffins $C_5–C_{11+}$	$W_5=k_5C_{isoparaffins}$	-
Cracking of olefins $C_5–C_{11+}$	$W_6=k_6C_{olefins}$	$W_{-6}=k_{-6}\ C^2_{gas}$
Hydrogen transfer	$W_7=k_7C_{olefins}\ C_{naphthenes}$	-
Dealkylation of naphthenes	$W_8=k_8C_{naphthenes}$	-
Dealkylation of aromatics	$W_9=k_9C_{aromatics}$	$W_{-9}=k_{-9}C_{monoaromatics}\ C_{olefins}$
Cracking polynaphthenes	$W_{10}=k_{10}C_{naphthenes}$	-
Condensation of aromatics	$W_{11}=k_{11}C_{aromatics}\ C_{olefins}$	-
Coke formation (polycondensation)	$W_{12}=k_{12}C_{resins}$	-
Cyclization of olefins	$W_{13}=k_{13}C_{olefins}$	$W_{-13}=k_{-13}\ C_{naphthenes}$
Dealkylation of monoaromatics	$W_{14}=k_{14}C_{monoaromatics}$	$W_{-14}=k_{-14}C_{monoaromatics}\ C_{olefins}$

Here the following paraffins HMW, naphthenes HMW, aromatics and resins – paraffins ($C_{13}–C_{40}$), high molecular weight naphthenes, aromatics, resins of raw materials; paraffins MMW, isoparaffins, olefins, naphthenes – paraffins, isoparaffins, olefins of gasoline fraction ($C_5–C_{11+}$);

The determination of kinetic parameters of reactions involves finding the reaction rate constants [22]. The determination of kinetic parameters and kinetic regularities of hydrocarbon conversion is determined by solving the inverse kinetic problem of the forward chaining method (tab. 3**)**.

Heat balance of catalytic cracking reactor is determined such parameters as the composition of raw materials, temperature and activity of the catalyst after regeneration stage. Amount of coke on the catalyst in the riser reactor depends on these parameters in a greater degree. Dynamics of coke accumulation determines the quantity of coke combustion during the regeneration and temperature of catalyst circulation and therefore, the process temperature, composition and yield of the light fractions from a catalytic cracking unit.

Table 3.Kinetic parameters of catalytic cracking reactions (T=794 K, Pressure=1.43 MPa)

Component	Reaction rate expression	
	direct reaction	reverse reaction
Cracking of paraffins C_{13}–C_{40}	$1.02 \cdot 10^{-1}$	
Cracking of paraffins C_{13}–C_{40} to isoparaffins	$6.92 \cdot 10^{-1}$	
Cracking of paraffins C_5–C_{11+}	$5.96 \cdot 10^{-3}$	
Isomerization of paraffins C_5–C_{11+}	$2.9 \cdot 10^{-4}$	$2.05 \cdot 10^{-4}$
Cracking of isoparaffins C_5–C_{11+}	$5.96 \cdot 10^{-3}$	
Cracking of olefins C_5–C_{11+}	$2.16 \cdot 10^{-1}$	
Hydrogen transfer	29.72	
Dealkylation of naphthenes	$5.82 \cdot 10^{-1}$	
Dealkylation of aromatics	$2.79 \cdot 10^{-1}$	
Cracking polynaphthenes	$7.64 \cdot 10^{-2}$	
Condensation of aromatics	$4.68 \cdot 10^{-1}$	
Coke formation (polycondensation)	$5.3 \cdot 10^{-1}$	
Cyclization of olefins	$5.79 \cdot 10^{-2}$	$1.86 \cdot 10^{-2}$
Dealkylation of monoaromatics	$4.31 \cdot 10^{-2}$	$4.00 \cdot 10^{-6}$

Catalyst raw materials ratio is defined from heat balance of catalytic cracking reactor [23].

$$\text{Cat/Raw materials} = \frac{Cp_S \times Gs \times (Tem - T_S) + H_R \times G_R + H_N \times G_N + \Delta H_{RM} + \Delta H_{CHR}}{Cp_C \times (T_{RC} - T_{RX})}$$

Program implementation of mathematical model was made using Delphi 7 software (fig. 3).

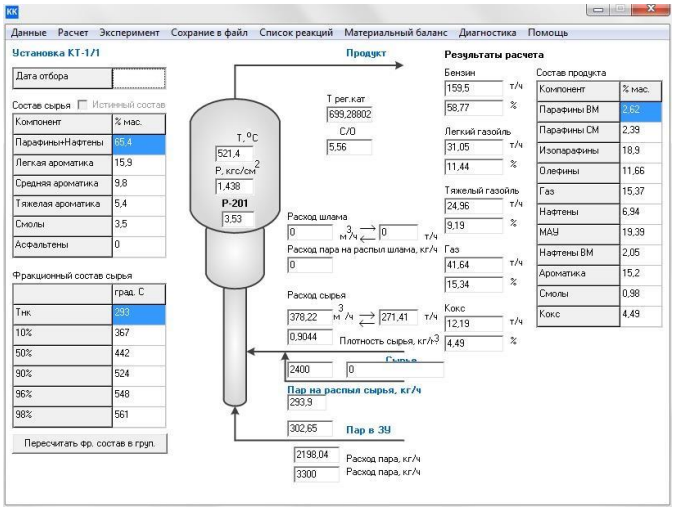

Figure 3. Active window of computer simulator of catalytic cracking

2.3. Model adequacy verification

The results of comparison of calculated and experimental values of main product yields are shown in tab. 4.

Table 4. Calculation error between calculation and experimental of product yields, %

Unit flow	Experimental value	Calculation value
Unstable gasoline	58.32	57.3
Light gasoil	11.46	11.61
Heavy gasoil	9.16	9.13
Rich gas	15.69	16.15
Coke	4.60	4.40
Loses	0.77	1.3
Temperature	521.0	520.66

Mathematical models of catalytic cracking also give a good convergence of experimental and calculated data. That's allowed to use a mathematical model as a computer simulator for training of effective exploitation of the catalytic cracking unit. Computer simulator "Catalytic Cracking" is designed to educate the efficient exploitation of industrial catalytic cracking unit and can be used on refineries and in the institution of higher education.

3. Results and discussion

3.1. Development of laboratory work and test control

Pedagogical design was made with using Adobe Dreamweaver CS 5.5 software. Methodological guidelines on discipline "Innovative Development of Chemical Technology of Natural Energy Resources" contain four laboratory works on oil refining. Laboratory work "Catalytic cracking" is performed using the author's computer modeling system.

The main program window of the electronic aid is presented in fig. 4.

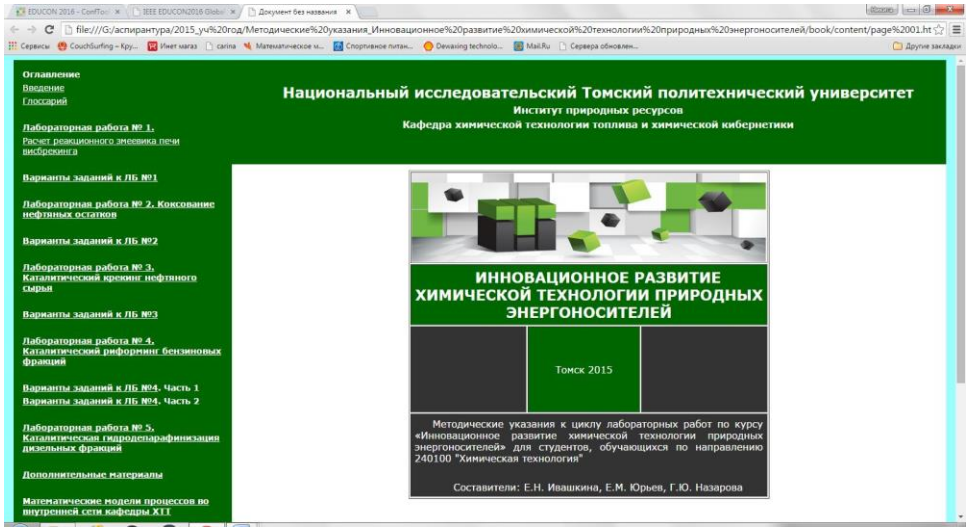

Figure 4. The main program window of the electronic aid

Laboratory work using computer modeling system aims to:

- it is a study of the theoretical foundations, physical and chemical irregularities, thermodynamic and kinetic irregularities of the catalytic cracking, operation features of the industrial unit.;
- it is solution of complex technological problems using experimental data from an industrial unit according to physical and chemical regularities of the process (prediction of the group composition, octane number and yield of gasoline from the catalytic cracking unit, evaluation the effect of the feedstock composition and technological mode on the yield of catalytic cracking products).

Innovative methods of pedagogical diagnostics are widespread among educators and focused on the identification and assessment of the competence level, accomplishments of students and their willingness to solve creative problems, the ability to logically and adequately build the text.

Testing method is one of the modern accurate and objective measurement methods for evaluation of student academic achievements and pedagogical tests which are used as measuring instrument [24].

Tests were developed in two directions: 1) test tasks aimed at assess in-depth knowledge in the oil refining field (in structure of the knowledge consolidation and self-control block); 2) test tasks aimed at assess the student achievements on the fundamentals of oil refining processes (final control). The final control is organized as follows: a solution of tests with followed by oral examination in the form of conversation. Such approach is aimed at students with a different types of the information perception, because test tasks can perceive more

difficult than oral examination for some category of students. They feel some worry during the testing and can't disclose the knowledge in full.

The developed complex of test tasks is focused on different levels the understanding of academic material and implemented using iSpring Suite 7 software (fig. 5).

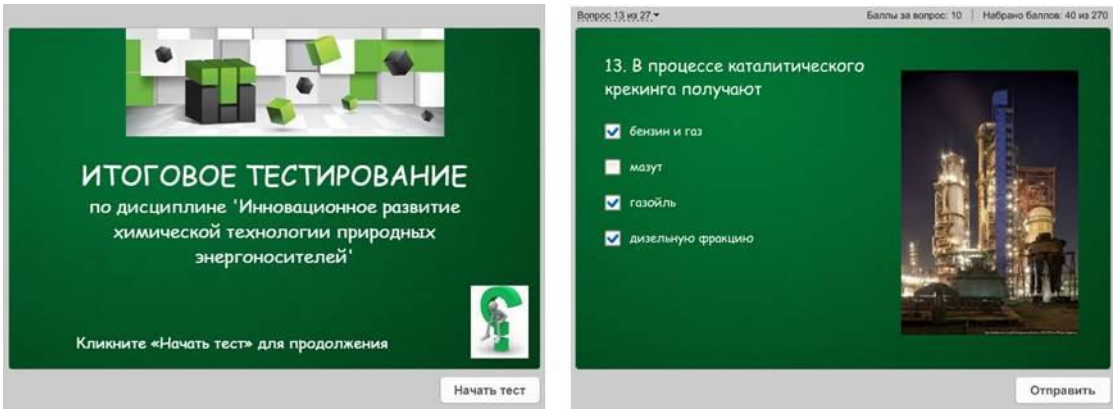

Figure 5. Example of test tasks

4. Conclusion

Specially trained and qualified staff are essential for complex oil refining processes because they bear a great responsibility for the consequences decisions by the management of the production. Using the dynamic modeling and computer simulators allows effectively organize educational process to the preparation of technologists for to effective operation the catalytic cracking unit.

Using upgraded electronic educational aid the students in the master's program "Chemical technology" can acquire not only basic but also in-depth knowledge and improve knowledge in the field of oil refining.

Electronic educational aid is aimed for students with various types of perception that provide the improve percentage of successful students. Methodological of guidelines to the laboratory works updated graphic elements, which makes it interesting and understandable for students with different backgrounds.

Developed methodological guidelines to the laboratory work appropriate the requirements to modern electronic educational aid and exhibits a practical importance. Students operate on the catalytic cracking mathematical model and work with experimental data from industrial unit and analyze regularities of the processes during the laboratory work. Such approach contributes to an active thought process.

Pedagogical design was made using the program Adobe Dreamweaver CS 5.5., Delphi 7 and ISpring Sute 7 software. Materials will be available in a computer lab of the profiling department and personal website of the teacher.

List of symbols

ΔG	*change in Gibbs energy of reaction, kJ/mole;*
ΔH	*change in Enthalpy of reaction, kJ/mole;*
C_i	*concentration of i-th hydrocarbon group, mole/m^3;*
W_j	*the rate of direct chemical reaction, mole/(m^3·sec);*
W_{-j}	*the rate of reverse chemical reaction, mole/(m^3·sec);*
kj	*the rate constant of direct chemical reaction;*
$k\text{-}j$	*the rate constant of the reverse chemical reaction;*
Cp_s	*specific heat of steam, kcal/kg^{o}C;*
G_s	*total consumption of steam in the riser, kg/h;*
Tem	*process temperature,^{o}C;*
T_s	*stream temperature, ^{o}C;*
H_R	*recycle to riser specific heat, kcal/kg;*

G_R *recycle consumption to riser, kg/h;*
H_N *lift gas enthalpy, kcal/kg;*
G_N *lift gas to riser, kg/h;*
ΔH_{RM} *heat consumed by raw materials, kcal/h;*
ΔH_{CHR} *heat of reaction, kcal/h.*

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