MATHEMATICAL MODELING AND SIMULATION OF POWER UNIT WORKING ON MOTOR FUELS DERIVED FROM NATURAL GAS IN TOTAL LIFE CYCLE

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ И РАСЧЕТНЫЕ ИССЛЕДОВАНИЯ ПОКАЗАТЕЛЕЙ СИЛОВОЙ УСТАНОВКИ, РАБОТАЮЩЕЙ НА МОТОРНЫХ ТОПЛИВАХ, ПОЛУЧЕННЫХ ИЗ ПРИРОДНОГО ГАЗА, В ПОЛНОМ ЖИЗНЕННОМ ЦИКЛЕ

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Abstract: *The article is devoted to the problem of comprehensive evaluation of the efficiency of the use of various alternative fuels obtained from natural gas (NG) in a total life cycle (TLC). Despite the fact that all types of motor fuel under consideration are produced from NG, the energy and environmental consequences of their use may vary significantly. Goals of this research are: developing TLC mathematical models of a power unit operating on motor fuels obtained from NG (compressed NG, liquefied NG, methanol, dimethyl ether, synthetic diesel fuel and hydrogen) and conducting a simulation in order to determine energy and environmental indicators for the use of the considered fuel types. The results of simulation allow to choose the most promising types of alternative fuels according to the criteria of energy efficiency and a level of environmental pollution by harmful substances and greenhouse gases.*

Key words: TOTAL LIFE CYCLE, MATHEMATICAL MODEL, ALTERNATIVE FUELS, NATURAL GAS, POWER UNIT

1. Introduction

Effective use of natural energy resources is important for the development of different industries and lowering of anthropogenic loads on environment and climate by lowering of emission of polluting substances and greenhouse gases. A special role in the solution of this problem is assigned to vehicles with engines powered by alternative types of fuel, first of all – by the natural gas (NG). [1,2,3]

Direct NG use, as well as obtaining other alternative motor fuels from NG, allows to increase the engine durability and the vehicle operation life by 1.3 - 1.5 times, to reduce the transportation prime cost by 15 - 25% due to a lower price of gas motor fuel, as well as to reduce essentially the harmful substance emissions to environment (carbon oxide – by 2.5 times, nitrogen oxides – by 2 times, hydrocarbons – by 3 times, smoke – by 9 times).

In many countries, the large-scale transport development programs are implemented in the direction of energy efficiency and environmental safety. The European Union (EU) is a leader on the matter. Thus, in 2011, the White Paper / Roadmap to a Single European Transport Area – Towards a Competitive and Resource Efficient Transport System (COM/2011/0144) was adopted suggesting that a share of used “standard-fueled vehicles” in public transport should be halved by 2030 and phased out in the cities by 2050.

The EU 2030 Climate and Energy Framework adopted in October 2014 sets the goals of lowering of greenhouse gas emissions by 40% in comparison with the level of 1990, achievement of renewable energy share up to 27%, as well as the resumption of activities aimed at the energy efficiency increase.

In the Russian Federation (RF), the main operating packages of legislation governing and providing to increase the use of motor fuels obtained from NG are as follows: the Russian Federation Government Order of 13.11.2009 No. 1715-r “Energy Strategy of Russia for the Period till 2030 (ES-2030)”; the Russian Federation Presidential Order of 17.12.2009 No. 861-rp “Climate Doctrine of the Russian Federation”; the Russian Federation Government Order of 13.05.2013 No. 767-r “On Expansion of Use of Natural Gas as Motor Fuel” (“On Regulation of the Relations in the Sphere of the Use of Gas Motor Fuel including NG as Motor Fuel”); the List of Instructions of Vladimir Putin, the President of the Russian Federation, following the meeting on prospects for using gas motor fuel of 24.06.2013 No. PR-1923; the Russian Federation Government Decree of 15.04.2014 No. 328 “On Approval of the State Program of the Russian Federation “The Development of Industry and Increase of its Competitiveness” (Main activity 1.7 “Expansion of Use of Natural Gas as a Motor Fuel”); the Russian Federation Government Decree of 07.12.2015 No. 1339 “On Amendments to the State Program of the Russian Federation “Energy Efficiency and Energy Development” and the Decree of the President of the Russian Federation of 01.12.2016 No. 642 “On the Scientific and Technological Development Strategy of the Russian Federation”.

Thus, a main goal of this research is the comprehensive evaluation of the efficiency of the use of various alternative fuels obtained from natural gas (NG) in a total life cycle (TLC) by development of TLC mathematical models of the power unit and carrying out of numerical analyses in order to determine energy and environmental indicators or parameters of the use of the considered fuel types.

At the TLC evaluation, the following fuel types are accepted: compressed natural gas (CNG), liquefied natural gas (LNG), methanol, dimethyl ether (DME), synthetic diesel fuel (DT) and hydrogen. It should be noted that environmental and energy consequences of the use of these types of motor fuels obtained from NG are different. It is explained by the fact that technologies of extraction of the fuels and routes of their distribution are significantly different.

2. The solution of the examined problem

Taking into account the known procedures for evaluation of power unit and fuel indicators or parameters in TLC and according to requirements of ISO 14040, ISO 14041, ISO 14042, ISO 14043 (in the Russian Federation - GOST R ISO 14040 - 14043) international standards, the mathematical models describing material and energy flows of the abovementioned motor fuels obtained from NG for stages of the power unit TLC were developed. At mathematical modeling, the following unit processes were considered: NG extraction, its transportation, NG compression, NG liquefaction, obtaining of synthesis gas, methanol, DME, synthetic DT, hydrogen, as well as obtaining of auxiliary fuels and electric energy necessary for the life cycle and the process of fuel use.

TLC of the power unit operating on the considered fuels includes three stages: fuel production, auxiliary processes and fuel use. For different types of motor fuels, the stages of auxiliary processes and fuel use, as well as a part of unit processes (NG extraction, NG transportation), will be identical as to the mathematical description.

This article shows the mathematical model of TLC of the power unit fueled by CNG in more detail. Mathematical models for other motor fuels considered in this research are not presented due to the limited volume of the article.

NG extraction process

Input flows

Amount of extracted NG (raw material) necessary for TLC, kg:

(1) $$M^{in}_{EXT,NG} = \left(1 + g_{EXT,NG}\left(\frac{1}{\eta_{EXT}} - 1\right)\right) M^{EXT}_{TRAN,NG},$$

where $g_{EXT,NG}$ is the NG consumption ratio for NG extraction process; η_{EXT} is the NG extraction process efficiency factor; $M^{EXT}_{TRAN,NG}$ is the NG amount at NG transportation process input, kg (see Formula 8).

Amount of auxiliary fuels at NG extraction process input, kg:

(2) $$M^{AUX.FUEL}_{EXT,aux.fuel} = \sum_i \left[\left(\frac{1}{\eta_{EXT}} - 1\right) g_{EXT,aux.fuel_i} \frac{Hu_{NG}}{Hu_{aux.fuel_i}} M^{EXT}_{TRAN,NG}\right],$$

where $g_{EXT,aux.fuel_i}$ is the i auxiliary fuel consumption ratio for NG extraction process; Hu_{NG} is the NG low heat value, MJ/kg; $Hu_{aux.fuel_i}$ is the i auxiliary fuel low heat value, MJ/kg.

Heat energy of NG (raw material) for NG extraction process, MJ:

(3) $$E^{in}_{EXT,NG} = Hu_{NG} M^{in}_{EXT,NG}.$$

Heat energy of auxiliary fuels for NG extraction process, MJ:

(4) $$E^{AUX.FUEL}_{EXT,aux.fuel} = \sum_i \left(M^{AUX.FUEL}_{EXT,aux.fuel_i} Hu_{aux.fuel_i}\right).$$

Electric energy for NG extraction process, MJ:

(5) $$E^{EL}_{EXT,el.en.} = \left(\frac{1}{\eta_{EXT}} - 1\right) g_{EXT,el.en.} Hu_{NG} M^{EXT}_{TRAN,NG},$$

where $g_{EXT,el.en.}$ is the electric energy consumption ratio for NG extraction process.

Output flows

Amount of harmful substance environmental emissions at NG extraction process, kg:

(6) $$M^{EXT}_{out,HE} = \sum_k \sum_i \left[\begin{array}{l} E^{AUXFUEL}_{EXT,aux.fuel_i} e_{i,k} + \\ + E^{in}_{EXT,NG}(1-\eta_{EXT}) g_{EXT,NG} e_{EXT,k} + M^{EXT}_{out,CH_4} \end{array}\right],$$

where $e_{i,k}$ is the k harmful substance specific emission at i auxiliary fuel burning in technological unit, kg/MJ; $e_{EXT,k}$ is the k harmful substance specific emission at NG burning at NG extraction process, kg/MJ; M^{EXT}_{out,CH_4} is the methane emission at NG extraction process, kg:

(7) $$M^{EXT}_{out,CH_4} = e_{EXT,CH_4} M^{EXT}_{TRAN,NG} Hu_{NG}.$$

Here, e_{EXT,CH_4} is the specific methane emission caused by process features and leaks, kg/MJ.

Amount of NG at NG transportation process input, kg:

(8) $$M^{EXT}_{TRAN,NG} = \left(1 + g_{TRAN,NG}\left(\frac{1}{\eta_{TRAN}} - 1\right)\right)\left(M^{TRAN}_{COMP,NG} + M^{TRAN}_{AUX.FUEL,NG} + M^{TRAN}_{EL,NG}\right),$$

where $g_{TRAN,NG}$ is the NG consumption ratio for NG transportation process; η_{TRAN} is the NG transportation process efficiency factor; $M^{TRAN}_{COMP,NG}$ is the NG amount at compression process input, kg (see Formula 19); $M^{TRAN}_{AUX.FUEL,NG}$ is the NG amount at auxiliary fuel obtaining process input, kg (see Formula 16); $M^{TRAN}_{EL.NG}$ is the NG amount at electric energy obtaining process input, kg.

NG heat energy for transportation process, MJ:

(9) $$E^{EXT}_{TRAN,NG} = Hu_{NG} M^{EXT}_{TRAN,NG}.$$

Heat energy environmental dissipation due to use of electric energy, the energy of combustion of auxiliary fuels and natural gas for NG extraction process, MJ:

(10) $$E^{EXT}_{out,en.to\,env.} = E^{EL}_{EXT,el.en.} + E^{AUX.FUEL}_{EXT,aux.fuel} + E^{in}_{EXT,NG}(1-\eta_{EXT}) g_{EXT,NG}.$$

NG transportation process

Amount of natural gas at NG transportation process input, kg, is determined from Formula 8.

Amount of auxiliary fuels at NG transportation process input, kg:

(11) $$M^{AUX.FUEL}_{TRAN,aux.fuel} = \sum_i \left[\left(\frac{1}{\eta_{TRAN}} - 1\right) g_{TRAN,aux.fuel_i} \frac{Hu_{NG}}{Hu_{aux.fuel_i}} M^{TRAN}_{COMP,NG}\right],$$

where $g_{TRAN,aux.fuel_i}$ is the i auxiliary fuel consumption ratio for NG transportation process.

NG heat energy for transportation process, MJ, is determined from Formula 9.

Electric energy for NG transportation process, MJ:

(12) $$E^{EL}_{TRAN,el.en.} = \left(\frac{1}{\eta_{TRAN}} - 1\right) g_{TRAN,el.en.} Hu_{NG} M^{TRAN}_{COMP,NG},$$

where $g_{TRAN,el.en.}$ is the electric energy consumption ratio for NG transportation process.

Heat energy of auxiliary fuels for NG transportation process, MJ:

(13) $$E^{AUX.FUEL}_{TRAN,aux.fuel.} = \sum_i \left(M^{AUX.FUEL}_{TRAN,aux.fuel_i} Hu_{aux.fuel_i}\right).$$

Output flows

Amount of harmful substance environmental emissions at NG transportation process, kg:

(14) $$M^{TRAN}_{out,HE} = \sum_k \sum_i \left[\begin{array}{l} E^{AUXFUEL}_{TRAN,aux.fuel_i} e_{i,k} + \\ + E^{EXT}_{TRAN,NG}(1-\eta_{TRAN}) g_{TRAN,NG} e_{TRAN,k} + M^{TRAN}_{out,CH_4} \end{array}\right],$$

where $e_{TRAN,k}$ is the k harmful substance specific emission at NG burning at NG transportation process, kg/MJ; M^{TRAN}_{out,CH_4} is the methane emission at NG transportation process, kg:

(15) $$M_{out,CH_4}^{TRAN} = e_{TRAN,CH_4} M_{COMP,NG}^{TRAN} Hu_{NG} .$$

Here, e_{TRAN,CH_4} a specific methane emission caused by process features and leaks, kg/MJ.

Amount of NG at auxiliary fuel obtaining process input, kg:

(16) $$M_{AUX.FUEL,NG}^{TRAN} = \sum_i \left[\left(1 + g_{AUX.FUEL,NG} \left(\frac{1}{\eta_{AUXFUEL_i}} - 1 \right) \right) \frac{\sum_j E_{j,aux.fuel_i}^{AUX.FUEL}}{Hu_{NG}} \right],$$

where $g_{AUX.FUEL,NG}$ is the NG consumption ratio for auxiliary fuel obtaining process; $\eta_{AUX.FUEL_i}$ is the i auxiliary fuel obtaining process efficiency factor; $E_{j,aux.fuel_i}^{AUX.FUEL}$ is the i auxiliary fuel heat energy for j process input, MJ:

(17) $$E_{j,aux.fuel}^{AUX.FUEL} = \sum_i (E_{EXT,aux.fuel_i}^{AUX.FUEL} + E_{TRAN,aux.fuel_i}^{AUX.FUEL} + E_{EL,aux.fuel_i}^{AUX.FUEL}),$$

where $E_{EL,aux.fuel_i}^{AUX.FUEL}$ is the i auxiliary fuel heat energy for electric energy obtaining process input, MJ:

(18) $$E_{EL,aux.fuel}^{AUXFUEL} = \sum_i \left(M_{EL,aux.fuel_i}^{AUX.FUEL} Hu_{aux.fuel_i} \right).$$

Amount of auxiliary fuels for electric energy obtaining process input, including NG, kg:

(19) $$M_{EL,aux.fuel}^{AUX.FUEL} = \sum_i \left[\left(1 + g_{EL,aux.fuel_i} \left(1 - \eta_{EL_i} \right) \right) \frac{E_{EL,aux.fuel_i}^{EXT}}{Hu_{aux.fuel_i}} \right],$$

where $g_{EL,aux.fuel_i}$ is the i auxiliary fuel consumption ratio for electric energy obtaining process; η_{EL_i} is the efficiency factor of electric energy obtaining process from i auxiliary fuel.

Amount of natural gas at NG compression and refueling process input, kg:

(20) $$M_{COMP,NG}^{TRAN} = \left(1 + g_{COMP,NG} \left(\frac{1}{\eta_{COMP}} - 1 \right) \right) M_{FU,mot.fuel}^{COMP},$$

where is the NG consumption ratio for NG compression and refueling process; η_{COMP} is the efficiency factor of NG compression and refueling process; $M_{FU,mot.fuel}^{COMP}$ is the amount of CNG at fuel use process, kg (see Formula 27).

Heat energy of NG at natural gas compression and refueling process, MJ:

(21) $$E_{COMP,NG}^{TRAN} = Hu_{NG} M_{COMP,NG}^{TRAN} .$$

Heat energy environmental dissipation due to use of electric energy, the energy of combustion of auxiliary fuels and NG for NG transportation process, MJ:

(22) $$E_{out,en.to\,env.}^{TRAN} = E_{TRAN,el.en.}^{EL} + E_{TRAN,aux.fuel}^{AUX.FUEL} + E_{TRAN,NG}^{EXT} (1 - \eta_{TRAN}) g_{TRAN,NG} .$$

NG compression and refueling process

Input flows

Amount of NG and heat energy of NG at NG compression and refueling process input shall be calculated according to Formula 20 and Formula 21 respectively.

Electric energy for NG compression and refueling process, MJ:

(23) $$E_{COMP,el.en.}^{EL} = \left(\frac{1}{\eta_{COMP}} - 1 \right) g_{COMP,el.en.} Hu_{NG} M_{FU,mot.fuel}^{COMP},$$

where $g_{COMP,el.en.}$ is the electric energy consumption ratio for NG compression and refueling process.

Output flows

Amount of harmful substance environmental emissions at NG compression and refueling process, kg:

(24) $$M_{out,HE}^{COMP} = \sum_k \sum_i \left[E_{COMP,NG}^{TRAN} (1 - \eta_{COMP}) g_{COMP,NG} e_{COMP,k} + M_{out,CH_4}^{COMP} \right],$$

where $e_{COMP,k}$ is the k harmful substance specific emission at NG burning at NG compression and refueling process, kg/MJ; M_{out,CH_4}^{COMP} is the methane emission at NG compression and refueling process, kg:

(25) $$M_{out,CH_4}^{COMP} = e_{COMP,CH_4} M_{FU,mot.fuel}^{COMP} Hu_{NG} .$$

Here, e_{COMP,CH_4} a specific methane emission caused by process features and leaks, kg/MJ.

Amount of CNG and heat energy of NG at fuel use process input shall be calculated according to Formula 27 and Formula 28 respectively.

Heat energy environmental dissipation due to use of electric energy, the energy of combustion and NG for NG compression and refueling process, MJ:

(26) $$E_{out,en.to\,env.}^{COMP} = E_{COMP,el.en.}^{EL} + E_{COMP,NG}^{TRAN} (1 - \eta_{COMP}) g_{COMP,NG} .$$

Fuel use process

Input flows

Amount of CNG at fuel use process input, kg:

(27) $$M_{FU,\,mot.fuel}^{COMP} = W m_{FU,CNG} ,$$

where W is the engine work, kWh; $m_{FU,CNG}$ is the specific CNG consumption per 1 kWh of a power unit operation, kg/kWh.

Heat energy of CNG, MJ:

(28) $$E_{FU,mot.fue;}^{COMP} = Hu_{CNG} M_{FU,mot.fuel}^{COMP} .$$

Output flows

Amount of harmful substance environmental emissions at fuel use process, kg:

(29) $$M_{out,HE}^{FU} = \sum_k W e_{FU,k} ,$$

where $e_{FU,k}$ is the k harmful substance specific emission at fuel use process per 1 kWh of power unit operation, kg/kWh.

Net energy (work) obtained from CNG use, MJ:

(30) $$E_{out,work}^{FU} = 3{,}6W .$$

Heat energy environmental dissipation due to use of CNG, MJ:

(31) $$E_{out,en.to\,env.}^{FU} = E_{FU,mot.fuel}^{COMP} - E_{out,work}^{FU} .$$

A mathematic model of TLC of the power unit working on CNG in total

Input flows

Raw material resources, kg:

(32) $$M^{in}_{TLC} = M^{in}_{FPS,NG} + M^{in}_{APS,raw}.$$

Energy, MJ:

(33) $$E^{in}_{TLC} = E^{in}_{FPS,NG} + E^{in}_{APS,raw}.$$

Output flows

Harmful substances, kg:

(34) $$M^{TLC}_{out} = M^{FPS}_{out,HE} + M^{APS}_{out,HE} + M^{FUS}_{out,HE}.$$

Energy to the environment, MJ:

(35) $$E^{TLC}_{out,en.to\,env.} = E^{FPS}_{out,en.to\,env.} + E^{APS}_{out,en.to\,env.} + E^{FUS}_{out,en\,to\,env.}.$$

Energy (useful work), MJ:

(36) $$E^{TLC}_{out,work} = E^{FUS}_{out,work}.$$

3. Results and discussion

There were numerical studies carried out based on the published inventory data and using the developed TLC mathematic model. [4,5] The calculation results for CNG are given in Figures 1-3. The TLC analyses for other motor fuel types are currently under development.

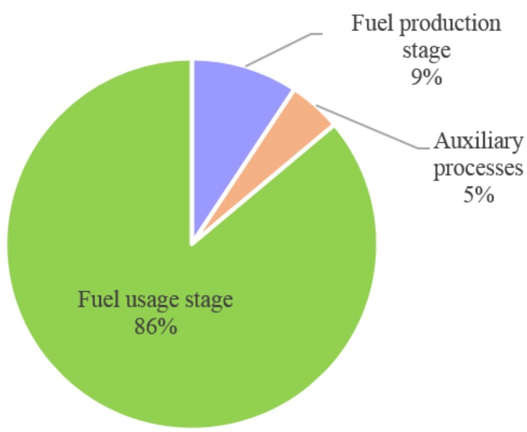

Fig. 1 *Structure of energy consumption throughout TLC by stages.*

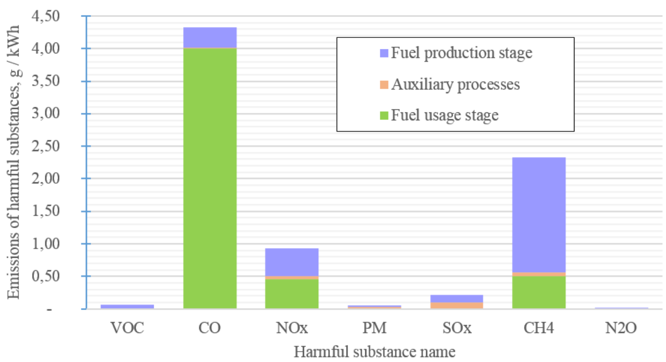

Fig. 2 *Structure of harmful substances emissions throughout TLC.*

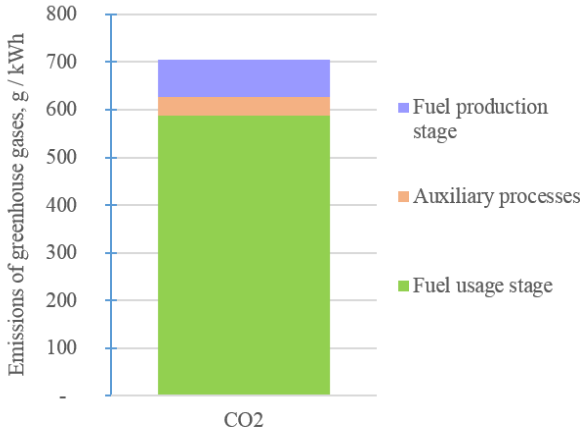

Fig. 3 *Structure of CO_2 emissions throughout TLC.*

4. Conclusion

Following the comprehensive effectiveness evaluation of the application of different alternative motor fuels obtained from NG, the following may be noted for the TLC:

- the developed mathematic models consider energy and material flows in the power unit TLC, consumption of natural resources and energy, harmful substances emissions to the environment;

- results of numerical analyses carried out using the developed mathematical model allow to compare and select the most promising types of alternative fuels according to the criteria of energy efficiency and a level of environmental pollution by harmful substances and greenhouse gases emission.

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