

# Integrated Methanol and Power Production Based On the Coal of the Tavan Tolgoi Coalfield

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**Abstract** — Mongolia has significant resources of high-quality coals. Because of the coal-fired TPP at the Tavan Tolgoi coalfield currently being designed, of greatest interest is the coal of the fourth seam of the Tavan Tolgoi coalfield with recoverable reserves of 6,500 million tons. The TPP is expected to offset the power shortage in the southern region of Mongolia as well as Tavan Tolgoi itself and the nearby Oyu Tolgoi mine. In light of the environmental requirements of today, new coal-fired power plants must be environmentally friendly and, if possible, produce additional marketable products along with electricity. For Mongolia, which imports all its liquid motor fuel, this could be methanol, which serves as a fuel for vehicles and the energy industry. This article investigates the issues involved in studying the competitiveness of the integrated production of methanol and electricity based on the coal of the Tavan Tolgoi coalfield in Mongolia.

**Index Terms:** co-generation, mathematical modeling, methanol, power generation.

## I. INTRODUCTION

Mongolia has significant resources of high-quality coals. Of most interest is the coal of the fourth seam of the Tavan Tolgoi coalfield that has recoverable reserves of 6 500 million tons. In terms of strategic importance, the Tavan Tolgoi coalfield is of great importance to the Mongolian economy, both for exports and for the creation and development of the coal processing industry and processing by coal chemical means.

There are plans to build a new coal-fired thermal

power plant at the Tavan Tolgoi coalfield, which should offset the power shortage in the southern district and Tavan Tolgoi itself and the nearby Oyu Tolgoi mine [9]. In light of the environmental requirements of today, new coal-fired thermal power plants must be environmentally friendly and, if possible, produce on-spec fuels with high added value along with electricity. For Mongolia, which is a net importer of liquid motor fuel, this could be methanol, which is a fuel for the energy industry serving the transport sector and the generation of heat and electricity. This article investigates the issues involved in studying the competitiveness of the integrated production of methanol and electricity based on the coal of the Tavan Tolgoi coalfield in Mongolia.

The conventional technology of methanol production from fossil fuels consists of two main steps: production of synthesis gas and synthesis of methanol from this gas. Both stages are characterized by the release of large amounts of heat, which is usually used to produce medium-pressure steam that is sent to the turbines that drive the compressors of the plant, as well as for the needs of other production facilities. This method of heat utilization is accompanied by significant losses during the operation. The combination of two processes – methanol synthesis and electricity generation at a single plant (combined-cycle gas turbine with integrated coal gasification and methanol synthesis, hereinafter referred to as CGMS-CCGT) – is a more efficient way to utilize the heat of gasification, as well as thermal and chemical energy of purge gases in the synthesis process. This combination improves energy efficiency, reduces investment by integrating the functions of some of the equipment, and streamlines the plant process flow diagram by eliminating the return flow of synthesis gas.

CGMS-CCGTs are characterized by high complexity of process flow diagrams, a variety of physical and chemical processes occurring in their components, as well as virtually no significant experience designing them. Mathematical modeling and modeled feasibility studies are the main way to study such plants.

A great deal of attention in the world is paid to research on technologies for converting fossil fuels into synthetic fuels [1, 2, 7]. The above studies have significant

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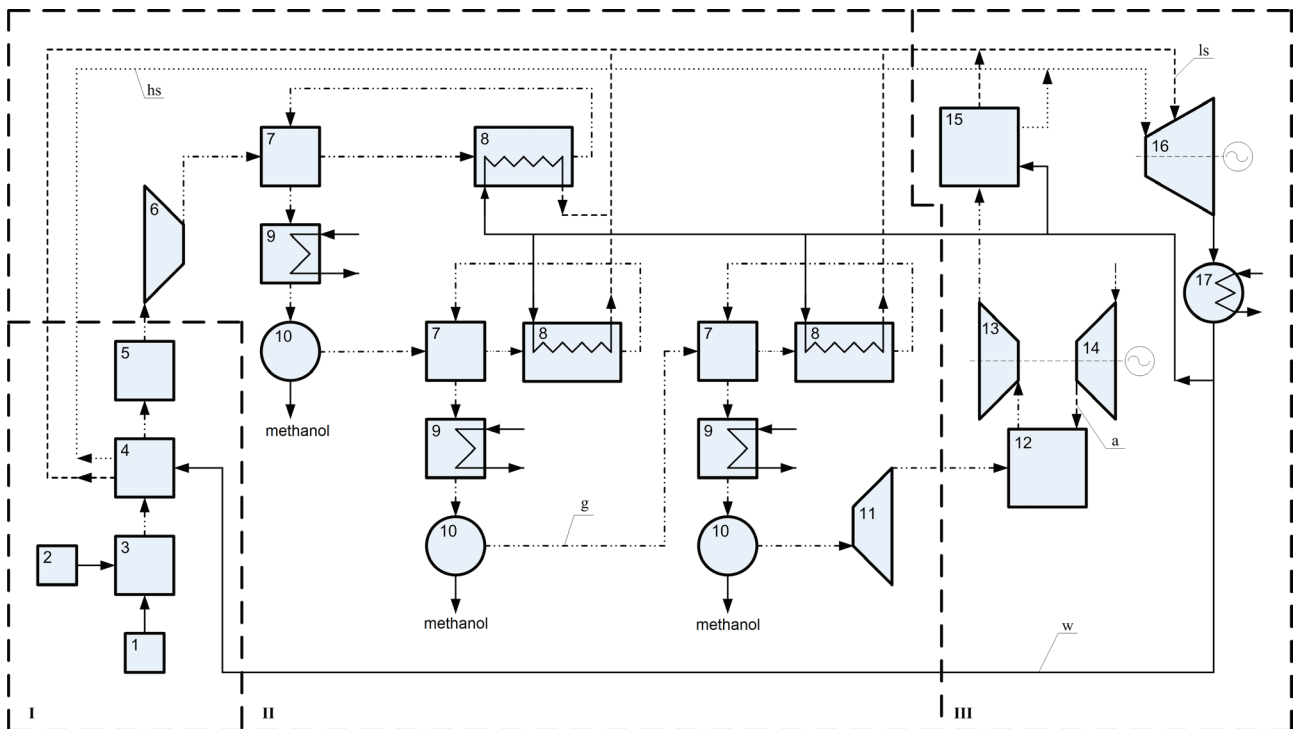
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**Fig. 1. CGMS-CCGT process flow diagram; g – gas, a – air, w – water, ls – low pressure steam, hs – high pressure steam; I – gasification unit, II – methanol synthesis unit, III – power unit; 1 – fuel preparation and supply system, 2 – oxygen generation system, 3 – gasifier, 4 – cooling system of gasification products, 5 – gasification product treatment system, 6 – synthesis gas compressor, 7 – regenerative gas-gas heat exchanger, 8 – methanol synthesis reactors, 9 – condenser, 10 – methanol separator, 11 – expansion turbine, 12 – gas turbine combustion chamber, 13 – gas turbine, 14 – air compressor, 15 – heat recovery steam generator, 16 – steam turbine, 17 – steam turbine condenser.**

differences, for ex-ample, in the layout of process flow diagrams, use of feedstock, conditions of plant operation, and methods for determining efficiency. This study is based on the methodology of systems re-search of complex fuel co-production power generation systems, based on comprehensive optimization studies backed by detailed mathematical models of the plant and its constituent elements.

## II. A METHODOLOGICAL APPROACH TO CGMS-CCGT STUDIES

The process flow diagram of the CGMS-CCGT was developed on the basis of state-of-the-art technologies. The process of fuel gasification is carried out in the reaction chamber of the gasifier in a fluidized bed at a pressure of 2 MPa. The optimal process flow diagram of methanol synthesis, with once-through synthesis reactors and intermediate cooling of synthesis products in heat exchangers by low-pressure steam was selected as a result of preliminary studies of various process solutions: with an isothermal reactor, with a primary synthesis reactor, with cooling of synthesis products by fresh synthesis gas, etc. The power generation unit provides for integrated gas-steam cycle, which is deemed the most promising for power plants (Fig. 1).

The CGMS-CCGT under consideration is a hybrid engineering system that includes both process and power

generation components of equipment with a complex layout of heterogeneous process links. The main way to study such plants is mathematical modeling and modeled numerical experiments. The models were developed using the SMPP software package developed at the Melentiev Energy Systems Institute, SB RAS [3]. This software package, based on information about the mathematical models of the individual elements of the units, the process links between them, and the purpose of calculation automatically generates a mathematical model of the unit in the form of a calculation program in the Fortran programming language.

The mathematical model of the gasification unit includes models of reaction chambers of gasifiers, freeboard, convective gas-water heat exchangers, and synthesis gas treatment system. The mathematical model of the methanol synthesis unit includes models of synthesis-gas compressors, catalytic reactor, regenerative gas-gas heat exchangers, and condensers. The mathematical model of the power unit includes models of the expansion and gas turbines, air compressor, purge gas combustion chamber, steam turbine compartments, steam turbine condenser, extraction stage heater, and heat recovery steam generator. The mathematical model of the CGMS-CCGT as a whole contains more than 2 000 parameters and hundreds of algebraic and transcendental equations. When developing mathematical models, various methods of mathematical

TABLE 1. Characteristics of the coal of the Tavan Tolgoi coalfield.

No.	Proximate analysis	Result	Limit value
1	Moisture content $W^r$ , %	10.5	4–17
2	Ash yield $A^r$ , %	24.8	10–33
3	Volatile matter $V^r$ , %	25.1	18–30
4	Sulphur $S^r_{total}$ , %		0.6–1.0
Ultimate analysis			
1	Carbon $C^{daf}$ , %	85.9	84–87
2	Hydrogen, %	5.15	2.0–6.7
3	Nitrogen, %	1.97	1.7–2.3
4	Sulphur, %	0.96	0.8–1.4
5	Oxygen, %	6	4.5–7.6
6	Chlorine, %	0.02	0.01–0.03
7	Calorific value	kcal/kg	5 000–6 300
8	$Q^r_H$	MJ/kg	18.5–26.0
Temperature points, °C			
1	Initial deformation temperature	1.08	1 050–1 600
2	Softening temperature	Sphere	1 100–1 600
3		Hemisphere	1 300–1 600
4	Flow temperature	1.35	1 300–1 600

programming were used [1, 3, 5, 6].

On the basis of the mathematical model of the CGMS-CCGT such engineering and economic performance metrics as the amount of methanol and electricity produced (at a given consumption of coal), plant efficiency, the mass of the catalyst for the synthesis, the area of heating surfaces of heat exchangers, capital expenditures, operating costs, etc. are determined.

In order to find the optimal options of the CGMS-CCGT structure it is necessary to solve the problems of non-linear programming, the purpose of which is to calculate the parameters of the plant so as to provide the minimum cost of methanol at a given internal rate of return, fuel and electricity price, while taking into account the physical and engineering constraints.

Mathematical problem statement

$$\min C_m(x, y, B, K, M, E, C_e, C_f, IRR_z)$$

subject to the following conditions

$$H(x, y) = 0,$$

$$G(x, y) \geq 0,$$

$$x_{min} \leq x \leq x_{max}$$

where  $C_m$  is the price of methanol,  $x$  is the vector of parameters to be optimized,  $B$  is the annual fuel consumption,  $K$  is capital expenditures of the CGMS-CCGT,  $M$  is the annual methanol production,  $E$  is the annual electricity production,  $C_e$  is the electricity price,  $C_f$  is the coal price,  $IRR_z$  is the internal rate of return,  $H$  is the vector of equation constraints,  $G$  is the vector of inequality constraints,  $x_{min}$ ,  $x_{max}$  are vectors of boundary values of the parameters to be optimized.

### III. ENGINEERING AND ECONOMIC OPTIMIZATION OF CGMS-CCGT PARAMETERS

The purpose of research conducted with the aid of mathematical models of the CGMS-CCGT is to determine the optimal parameters of the plant and the sensitivity of its economic performance to changes in external conditions. This is required to assess the prospects for large-scale application of this method of processing the coal of the Tavan Tolgoi coalfield.

The ratio between methanol synthesis and electricity generation has the greatest effect on the engineering and economic performance of the plant. The main parameters affecting this ratio are the composition of the blast into the gasifier, which determines the composition of the synthesis gas, and the number of reactors in parallel in the stages of the synthesis unit, which determines the degree of conversion of the synthesis gas into methanol. Note that the amount of oxygen for gasification was determined assuming that the required gasification temperature for a given steam flow rate is ensured. In this paper, we consider different options of the CGMS-CCGT with different values of the above parameters.

The main input data, which were taken for the analysis of the CGMS-CCGT process flow diagram and calculation of its engineering and economic performance metrics, were assumed on the basis of cost estimates of CCGTs and chemical plants for methanol synthesis, taking into account the uncertainty of capital expenditures [9].

Table 1 shows the characteristics and composition of

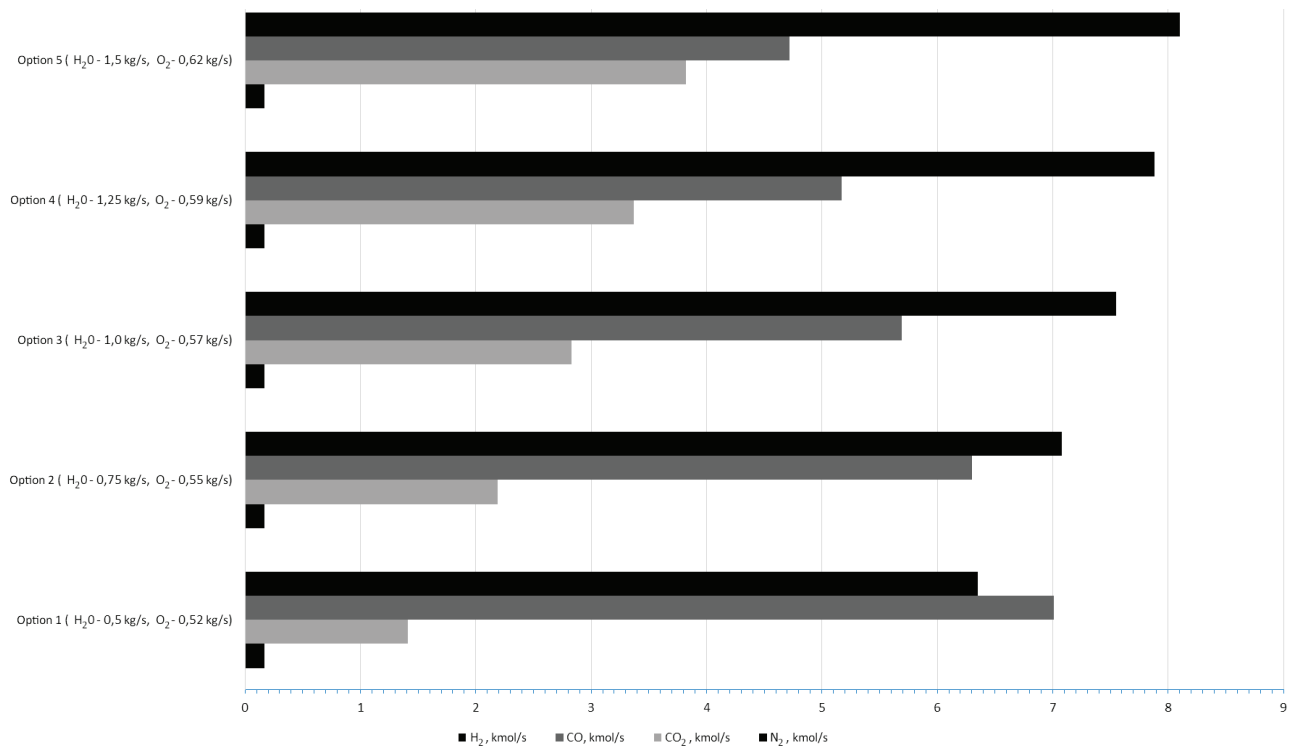


Fig. 2. Compositions of synthesis gas for each CGMS-CCGT option.

TABLE 2. Optimal values of engineering and economic performance metrics of the fuel co-production power generation system.

Metric	Option 1	Option 2	Option 3	Option 4	Option 5
Annual consumption of oil equivalent, thousand t.c.e.			3 500		
Methanol synthesis catalyst consumption, tons/year	450 441.5	392 435.2	338 558.0	302 170.7	280 904.0
Capacity, MW:					
air compressor	399.6	314.0	261.8	226.5	237.1
oxygen compressor	37.6	39.4	41.0	44.2	42.5
synthesis gas compressor	61.2	61.2	60.6	58.8	59.8
Gas turbine capacity, MW	681.5	541.0	455.6	397.3	415.1
Steam turbine capacity, MW	362.1	357.2	360.4	385.5	370.7
Expansion turbine capacity, MW	16.4	13.7	12.2	11.1	11.4
Net capacity, MW	408.9	340.2	303.3	293.3	291.6
Auxiliary capacity, MW	651.1	571.8	524.9	500.7	505.7
Annual electricity generation, mln. kWh	2 862.4	2 381.1	2 123.1	2 051.1	2 042.8
Annual methanol production, thousand tons (thousand t.c.e.)	1 709.3 (1 231.9)	1 878.5 (1 353.8)	1 947.9 (1 403.9)	1 951.1 (1 406.2)	1 920.9 (1 384.4)
Capital expenditures of the plant, thous. US dollars.	1 404.82	1 344.13	1 320.09	1 339.65	1 341.35
inclusive of the following:					
gasification unit	439.91	454.72	467.80	480.55	494.06
synthesis unit	479.87	458.61	452.03	472.04	461.63
power unit	485.05	430.80	400.26	387.06	385.66
Thermal efficiency, %	0.620	0.650	0.657	0.653	0.644
Methanol price, US doll. /t.c.e.	416	377	368	375	382

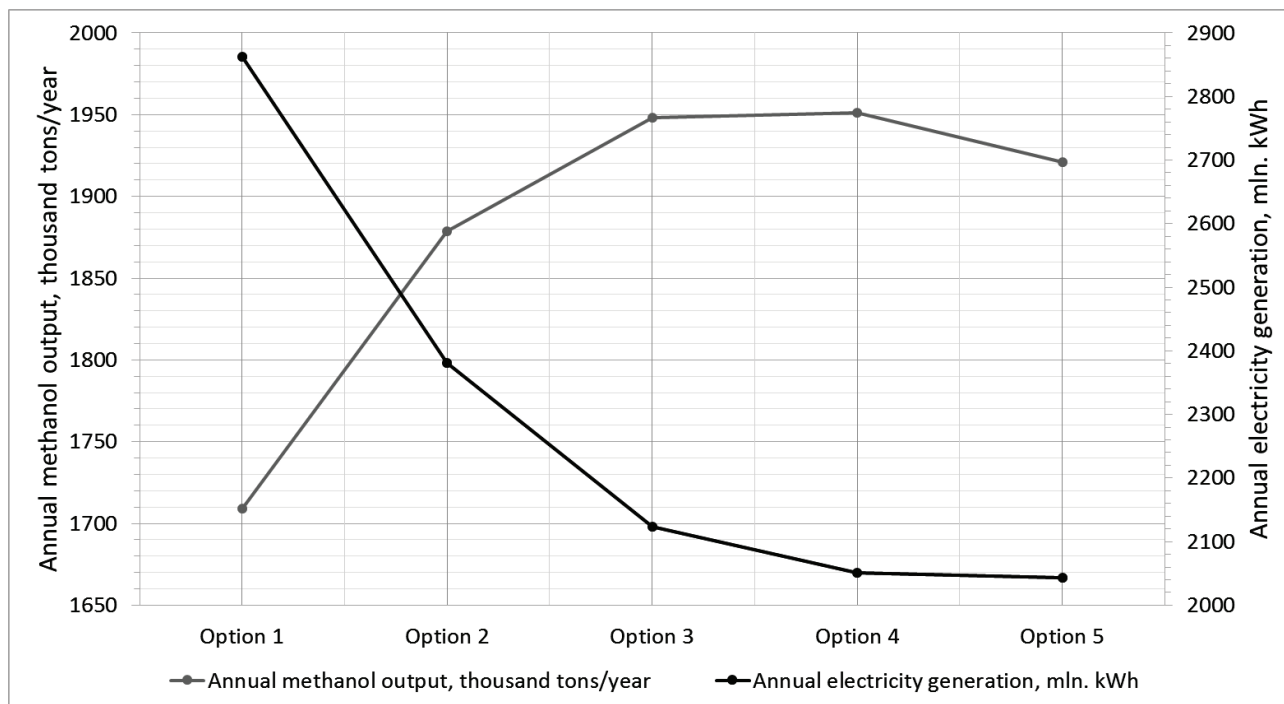


Fig. 3. Annual output of methanol and electricity.

the coal of the Tavan Tolgoi coalfield of Mongolia. Figure 2 shows the investigated options of the CGMS-CCGT that are characterized by different composition of the gasifying agent and compositions of synthesis gas obtained as a result of gasification of coal of the Tavan Tolgoi coalfield.

The optimal values of engineering and economic performance metrics for the options under study are presented in Table 2.

Figure 3 shows the ratio of annual electricity to methanol output for each option.

#### IV. CONCLUSION

In terms of economic performance (minimum price of produced methanol) and energy efficiency (maximum thermal efficiency of methanol production) it is Option 3 that proves optimal.

It can be seen that the CGMS-CCGT has a high thermal efficiency: up to 66% as compared to 55% for conventional coal-fired methanol synthesis plants. Option 1 having the lowest specific steam consumption for blast is characterized by minimum methanol production and maximum electricity generation. This is due to the lack of hydrogen in the synthesis gas, which is necessary for the formation of methanol. Significant amounts of CO remaining after the synthesis reactions enter the combustion chamber of the gas turbine, resulting in increased power generation. However, the increase in revenue from electricity production fails to offset the growth of capital expenditures, and the price of methanol is at its maximum. Option 5 that comes with the highest steam consumption is characterized by the lowest electricity production and sufficiently high methanol output.

Option 3, which is deemed optimal, is characterized by a significant deviation of the composition of fresh synthesis gas from the one required stoichiometry-wise (the  $H_2:CO$  ratio is lower). Working with this composition reduces energy losses, and all excess CO is burned off in the power plant. This circumstance makes it possible to abandon the expensive CO conversion unit, reduce the supply of water steam into the gasifiers (compared to dedicated methanol synthesis plants), which increases the energy efficiency of the use of chemical energy of coal. It should be noted that due to greater slip stream of gas from the synthesis unit (significantly greater than that for methanol synthesis process units), the productivity of synthesis reactors increases dramatically (approximately twofold), because they operate on synthesis gas with a more favorable composition.

Another important defining feature of the CGMS-CCGT is its environmental friendliness. This is due to the following circumstances. Hydrogen sulfide content in the synthesis gas entering the synthesis unit must not exceed  $0.2 \text{ mg/nm}^3$  (as per the requirements imposed by the catalyst) and ash content must not exceed  $5 \text{ mg/nm}^3$  (as per the requirements of preventing erosion of the flow channel part of gas compressors and turbines). As for nitrogen oxides, their only source is the combustion chamber of the gas turbine of the power unit. This is hundreds of times less in terms of  $SO_2$ , 2 times less in terms of ash, and 4 times less in terms of  $NO_x$  than the environmentally friendly thermal power plants.

In the range of methanol prices from 416 to 368 US dollars / t.c.e., obtained for each CGMS-CCGT option while taking into account the projections of changes in

world oil prices and trends in the ratio of oil prices to prices of other fuels, we can conclude that methanol produced from the coal of the Tavan Tolgoi coalfield can successfully compete with methanol produced at conventional dedicated methanol synthesis plants.

There is a fairly large set of plausible combinations of economic conditions under which methanol and electricity production plants prove economically viable. Therefore, these plants are promising and require more detailed study, primarily through the construction of pilot plants.

#### REFERENCES

- [1] A. V. Fiacco, G. P. McCormick, *Nonlinear Programming: Sequential Unconstrained Minimization Techniques*. New York, NY, USA: Wiley and Sons, 1968.
- [2] Y. Jiang, D. Bhattacharyya, “Techno-economic analysis of direct coal-biomass to liquids (CBTL) plants with shale gas utilization and CO<sub>2</sub> capture and storage (CCS),” *Applied Energy*, vol. 189, pp. 433–448, 2017.
- [3] A. M. Kler, A. S. Maximov, E. L. Stepanova, “Mathematical modeling and optimization of large thermal power installations,” in *Proceedings of the ASME-ATI-UIT 2010 Conference Thermal and Environmental Issues in Energy Systems*, Italy, Sorrento, 2010, pp. 391–400.
- [4] G. Liu, Z. Li, M. Wang, W. Ni, “Energy savings by co-production: A methanol/electricity case study,” *Applied Energy*, vol. 87, pp. 2854–2859, 2010.
- [5] J. Martín-Vaquero, B. Kleefeld, “Extrapolated stabilized explicit Runge–Kutta methods,” *Journal of Computational Physics*, vol. 326, pp. 141–155, 2016.
- [6] L. Skvortsov, “Explicit stabilized Runge-Kutta methods,” *Computational Mathematics and Mathematical Physics*, vol. 51, pp. 1153–1166, 2011. DOI: 10.1134/S0965542511070165.
- [7] J. Zhang, L. Ma, Z. Li, W. Ni, “The impact of system configuration on material utilization in the coal-based polygeneration of methanol and electricity,” *Energy*, vol. 75, pp. 136–145, 2014.
- [8] B. Bat-Erdene, S. Batmunkh, N. I. Voropai, V. V. Khanaev, P. S. Drachev, “Development of the Mongolian energy industry: II. Revisiting the issue of modeling and optimization of the IPS structure,” *Energy & Engineering*, no. 2(204), pp. 21–32, 2021.
- [9] A. M. Kler, N. P. Dekanova, E. A. Tyurina, *Heat and power systems. Optimization Studies*. Novosibirsk, Russia: Nauka, 2005, 236 p.