Biomass conversion into synthetic liquid fuel and electric energy: comparison of prospective technologies

E A Tyurina\textsuperscript{1,2}, A S Mednikov\textsuperscript{1}, P Yu Elsukov\textsuperscript{1}, S N Sushko\textsuperscript{2}

\textsuperscript{1}Melentiev Energy Systems Institute SB RAS, 130 Lermontov str., Irkutsk, Russia
\textsuperscript{2}Irkutsk National Research Technical University, 83 Lermontov str., Irkutsk, Russia

E-mail: tyurina@isem.irk.ru

Abstract. Based on an analytical review, a scheme of a unit for dimethyl ether (DME) synthesis based on woody biomass was selected and its mathematical model was developed. The model adequately reflects the thermodynamic processes that occur in the components of the unit. It is included in the model of a power plant for combined DME and electricity production. The mathematical model of the plant was used to investigate different options of gasification agent. The DME synthesis plant was compared with the methanol synthesis plant investigated earlier in terms of a complex economic index – internal rate of return. The findings demonstrate that the selling price of electricity generated from these plants plays an essential part in the determination of the efficiency area of the methanol or DME synthesis plants.

1. Introduction
The interest in the energy use of biomass has revived lately. This is explained by the influence of several main factors: rising prices for fossil fuels, which are considered as a threat to energy security; global climate change; and the adoption of international commitments to reduce greenhouse gas emissions. The use of biomass as an energy resource in remote areas of Siberia and the Far East where the imported energy fuel is very expensive and the reserves of low grade woody biomass are large, becomes especially important in the context of Russia.

Three main areas of biomass energy use may be highlighted: direct combustion to produce heat and electricity; gasification to produce combustible gases which are burnt to produce heat and electricity, and production of synthetic liquid fuels.

The paper considers a promising direction for biomass processing. This is the oxidative conversion of this raw material to produce gas enriched with hydrogen and carbon oxides. Pre-cleaned gas can be considered as synthesis gas for production of valuable synthetic liquid fuels (SLF). The synthetic liquid fuels are, first of all, the environmentally friendly energy carriers such as methanol and DME, which can be used not only as energy but also as motor fuels [1, 2].

The oxidative conversion of biomass and the possible conversion of synthesis gas into chemical products are characterized by release of a large amount of heat and carbon oxides [2, 3]. The combination of chemical processes with the electricity generation enhances the efficiency of waste processing. An analysis of technologies for processing various organic raw materials, which was made at the Melentiev Energy Systems Institute SB RAS, revealed the feasibility of combining the
technology for chemical processing with electricity generation [3]. The energy and economic efficiency of such an integrated technology is considerably higher than that of separate productions. The findings of the research into the combined production of methanol and electricity from woody biomass are presented in previous papers by the authors. The objective of this study is to optimize technical and economic indices of the combined production of DME and electricity at power plants in order to obtain optimal solutions. They have to be taken into account in the energy balances of remote areas of the Russian Federation.

Let us note some characteristics of DME as a fuel. Although the calorific value of DME is 1.5 times lower than that of traditional diesel fuel, it is superior in other properties: the most important characteristic of diesel fuel is the cetane number which is 55-60 for DME versus 40-55 for diesel fuel, and the ignition temperature of DME is 235 °C versus 250 °C for diesel fuel. These features simplify the start of a cold engine, and the presence of oxygen in the DME composition provides smokeless combustion of the fuel. Moreover, the engine running on DME produces virtually no noise. The main advantage of DME as diesel fuel is an exhaust which meets the most stringent environmental requirements in the world (EURO and ULEV) without any purification [4].

2. Flow diagram of a modular power plant (MPP)

The focus of the paper is modular power plants for combined DME and electricity productions, which represent integrated technical systems with the components (devices) of both DME synthesis plants and IGCC. Modular power plants can be divided into three subsystems (blocks): the woody biomass gasification, the DME synthesis and power production. The processes that occur in the gasification subsystem are steam-air gasification of woody biomass, cooling and purification of gasification products, and generation of high and low pressure steam. The catalytic synthesis of dimethyl ether is carried out in the synthesis subsystem. The heat exchangers located between the catalyst zones of synthesis reactors generate low-pressure steam. It goes to the energy subsystem to generate power. In the energy subsystem the unreacted gas from the synthesis block is burnt, the high and low pressure steam is generated in the waste heat boiler, and electricity is generated in steam and gas turbines. The capacity of biomass processing plants can be built up, as required, by compact modular units. Biomass is gasified in fluidized bed gasifier with steam-air gasification agent under a pressure of 2 MPa and dry slag removal. Such gasifiers are most often used in the SLF synthesis plants. The DME synthesis has one stage. Electricity is generated in the IGCC. The flow diagram of the MPP is shown in figure 1.

Most of the studies of such complex systems as the modular power plant for combined generation of electricity, heat and SLF in Russia and other countries (Mobil, Cortus Energy, DTU, Lurgi Energie, ICT RAS, etc.) are devoted to the study of individual processes and devices. Complex studies on the technologies for generation of electricity and heat and synthesis of SLF mainly focus on economic and thermodynamic analyses. This work is dedicated to optimization studies of MPPs which are based on detailed models of energy and production process given the non-linearity of the occurring processes.

3. Mathematical modeling of MPP

Note that there are mathematical models developed previously for most of the energy components of MPP [3, 4]. A totally new component is a catalytic reactor for DME synthesis. In contrast to methanol synthesis, for the technologies of catalytic DME synthesis from synthesis gas, the equations of chemical kinetics of these processes are not given in available publications. Their authors only point out high selectivity and performance of these technologies. Therefore, the mathematical model of DME synthesis reactors relies on the equilibrium thermodynamics relationships in the article.

Determination of the equilibrium composition of the gas mixture during an isobaric-isothermal process is reduced to minimize the Gibbs function
(a) gas flows, (b) air, (c) feedwater flows, (d) high-pressure steam flows, (e) low-pressure steam flows, (f) methanol recirculation; I- gasification unit; II – DME synthesis unit; III – power production unit; 1-fuel-preparation system, 2-air separation system, 3-gasifier, 4- convective gas generator shaft, 5-gasification product cleaning system, 6-synthesis gas compressor, 7-regenerative gas-gas heat exchanger, 8 - catalytic synthesis reactors, 9- condenser, 11-expansion turbine, 12- purge gas combustion chamber, 13-main gas turbine, 14-air compressor, 15-heat recovery boiler, 16-steam turbine, 17-steam turbine condenser, 18- unit for separation of water, methanol, and DME.

Figure 1. Flow diagram of an MPP:

\[
\begin{align*}
\min & \quad G(T_{\text{out}}, P_{\text{out}}, y_1^{\text{out}}, \ldots, y_J^{\text{out}}) \\
\text{subject to} & \quad \delta_i^M = \sum_{i=1}^{L} K_i \cdot y_i^{\text{in}} - \sum_{j=1}^{J} K_j \cdot y_j^{\text{out}} = 0, \quad i = 1, \ldots, I,
\end{align*}
\]

where \( T_{\text{out}} \) is the temperature of gas mixture at reactor inlet and outlet, \( P_{\text{out}} \) is the pressure of gas mixture at reactor outlet, \( y_i^{\text{in}} \) is the molar flow rate of the \( i \)-th component of gas mixture at reactor inlet, \( L \) is the the number of gas mixture components at reactor inlet, \( y_j^{\text{out}} \) is the molar flow rate of the \( j \)-th components of gas mixture at reactor outlet, \( J \) is the number of gas mixture components at reactor outlet, \( K_i \) is the number of moles of the \( i \)-th chemical element, that are contained in one mole of the \( i \)-th chemical element that are contained in one mole of the \( j \)-th component of the output mixture, and \( I \) is the number of chemical elements.

A solution to this problem is a stationary point of the Lagrange function

\[
L(y, u) = G(T_{\text{out}}, P_{\text{out}}, y_1^{\text{out}}, \ldots, y_J^{\text{out}}) - \sum_{i=1}^{L} u_i - K_i(y_j),
\]

where \( u_i \) is the Lagrange multiplier related to the equality constraint \( \delta_i^M = 0 \).

The temperature of the synthesis products at the reactor outlet is determined from the condition of the energy balance.

To develop effective mathematical models of the modular power plant, we have created a design scheme of the plant. It differs from the technological plant by that its each component should have a mathematical model, and each technological link between the components of the scheme should correspond to data communication between the models. The mathematical model of the modular power plant was built using the software SCAGP developed by a research team of the Melentiev Energy Systems Institute, Siberian Branch of the Russian Academy of Sciences, and successfully applied in the simulation and optimization studies of thermal power plants. Based on the information about the mathematical models of individual components, technological links between them and the calculation purposes, the SCAGP automatically generates a mathematical model of the MPP as a calculation program in the Fortran. The model of the modular power plant contains about 2000 variables, and several hundreds of algebraic and transcendental equations. The iterative Gauss–Seidel method is used to solve the system of equations defining the individual units and the entire plant.
The mathematical model of MPP is intended for the design-calculation of the plant components: determination of heating surfaces of heat exchangers, catalyst volume in reactors, drive power of pumps and compressors, power of gas and steam turbines, flow rates and thermodynamic parameters of synthesis gas, products of combustion, gasification products, water, steam, steam-water mixture at various points of the scheme.

4. Results of technical-economic studies of the MPP

Note that there are mathematical models developed previously for most of the energy components of MPP [3]. A totally new component is a catalytic reactor for DME synthesis. In contrast to methanol synthesis, for the technologies of catalytic DME synthesis from synthesis gas, the equations of chemical kinetics of these processes are not given in available publications. Their authors only point out high selectivity and performance of these technologies. Therefore, in this paper, the development of a mathematical model of DME synthesis reactors relies on the equilibrium thermodynamics relationships.

The aim of the studies conducted using the mathematical models of MPP is to determine the optimal parameters of the plant and the sensitivity of its economic indices to changes in the external conditions. This is required to assess the prospects for the application of this method of woody biomass processing.

An analysis of the flow diagrams of MPP has revealed that the main factor that affects the cost of all units of the plant, its thermal efficiency and technical and economic indices is the relationship between the production of DME and the generation of electricity. The main parameter that influences this relationship is the consumption of steam and air as gasification agents, which determines the composition of synthesis gas. Note that in the calculations, the gasification process temperature was set, and consumption of air as a gasification agent was determined from the condition of ensuring the required gasification temperature for a given steam consumption. Thus, an independent parameter determining the relationship between the production of DME and the generation of electricity is the specific consumption of steam as a gasification agent.

It is worth noting that since the use of both DME and methanol as SLF is promising, which was indicated earlier, it is of interest to compare their production technologies in equal economic conditions. Therefore, to implement the most important principle of comparability of the studied options of the modular power plant, non-linear optimization of its basic parameters is carried out, subject to constraints.

Statement of the optimization problem of the MPP parameters

$$\min_{dW, dD} C_{DME} (x, y, dB, dW, KI, P_{DME}, P_{el}, c_w, c_{el}, IRR_z),$$

subject to

$$H(x, y) = 0, G(x, y) \geq 0, x_{min} \leq x \leq x_{max}, IRR = IRR_z,$$

where $x$ is the vector of independent optimized parameters; $y$ is the vector of dependent calculated parameters; $H$ is the vector of equality constraints; $G$ is the vector of inequality constraints; $x_{min}, x_{max}$ is the vector of boundary values of the optimized parameters; $dB, dD$ is the specific (per 1 kg of biomass) consumption of steam and air as gasification agents; $C_{DME}$ is the DME price; $B_w$ is the annual biomass consumption; $KI$ is the capital investment in MPP; $P_{el}$ is the annual electricity production; $P_{DME}$ is the annual DME production; $c_w$ is the biomass price; $c_{el}$ is the generated electricity price; and $IRR_z$ is the set internal rate of return.

The enthalpies, pressures and flow rates of high- and low-pressure steam, the volume of catalyst in the synthesis reactor, etc. were assigned as parameters to be optimized. The system of constraints includes the constraints on non-negativity of end-to-end temperature differences of heat exchangers, pressure drops along the flow path of steam and gas turbines; on design temperatures and mechanical stresses of heat exchanger pipes, on minimum and maximum gasification temperatures, etc. The initial technical and economic information was taken from the research done at the Melentiev Energy Systems Institute and focused on the conversion of solid fuel into synthetic liquid fuel and an analysis
of cost estimates of technological and energy production taking into account the operating conditions of MPP [3]. The price of biomass is 50 US$/tce, the selling price of electricity is 6.5 cents/kWh, and the gasification temperature is 1273 K. The internal rate of return is 15%. The composition of woody biomass is: C = 0.443, H = 0.055, S = 0.003, O = 0.14, N = 0.004, H₂O = 0.1, A = 0.047, and the lowest calorific value is 17 MJ/kg.

Some parameters of optimal options of the power plant are presented in table 1. The final technical and economic indices of the compared technologies are given in table 2.

### Table 1. Optimal parameters of MPP options.

| Name, unit of measurement | Plant for synthesis of | Methanol | DME |
|---------------------------|-----------------------|---------|-----|
| Specific air consumption for woody biomass gasification, kg/kg of fuel | | 0.79 | |
| Specific steam consumption for woody biomass gasification, kg/kg of fuel | | 0.6 | |
| Yield of gasification products, (kg/s): | | | |
| hydrogen | | 0.79 | |
| carbon oxide | | 8.9 | |
| carbon dioxide | | 6.0 | |
| water steam | | 5.1 | |
| nitrogen | | 13.9 | |
| Flow rate of methanol or DME from separators, kg / s: | | | |
| first synthesis stage | 3.2 | 3.6 | |
| second synthesis stage | 1.46 | 1.3 | |
| third synthesis stage | 0.82 | 0.4 | |
| Purge gas mass flows of the third synthesis stage, kg/s: | | | |
| hydrogen | 0.55 | 0.09 | |
| carbon oxide | 0.81 | 0.02 | |
| carbon dioxide | 0.57 | 1.72 | |
| water steam | 5.4 | 1.44 | |
| methanol | 0.4 | 0.001 | |
| DME | | | |
| nitrogen | | | 0.22 |
| Live steam flow rate in steam turbine, kg/s | 15.5 | 8.6 | |
| Low-pressure steam flow rate in steam turbine, kg/s | 23 | 18.4 | |
| Power, MW: of steam turbine | 21.5 | 15.1 | |
| of main gas turbine | 19.3 | 6.3 | |
| Auxiliary power, MW | 17.8 | 18.5 | |
| Useful electric power of the plant, MW | 23.5 | 6.0 | |

### Table 2. Main technical and economic indices of MPP.

| Indices | MPP for synthesis of |
|---------|---------------------|
| | Methanol | DME |
| Annual consumption of natural fuel, million t | 320 | |
| Annual consumption of fuel equivalent, thousand tce. | 200 | |
| Annual production of methanol or DME in fuel equivalent, thousand tce. | 99.6 | 128.1 |
| Annual production of methanol or DME, kt | 138.2 | 130.0 |
| Annual electricity output, million kWh | 165.1 | 41.0 |
| Capital investment in the plant, million USD | 112.6 | 119.8 |
| Thermal efficiency of methanol or dimethyl ether production, % | 66.2 | 68.3 |
| The SLF price (15%), USD / tce. | 376 | 395 |
5. Discussion of results

The Tables show that the optimal composition of synthesis gas for synthesis of DME and methanol is observed under the same composition of gasification agents. In this case, the CO/H\textsubscript{2} ratio is the highest, which contributes to an increase in the SLF production.

The optimal MPP option for the production of dimethyl ether is characterized by significantly lower power generation and considerable consumption of auxiliary power. This is because almost all CO is consumed in synthesis reactors for DME production. In the methanol synthesis plant, a considerable amount of CO goes to the combustion chamber of gas turbine after synthesis.

Methanol production has a higher thermal efficiency of synthesis. The plant of DME synthesis has lower capital investment due to the lower production of electricity and, accordingly, lower capital investment in the power generation block.

Comparison of the plants on the complex economic index, i.e. internal rate of return, has shown that the selling price for electricity produced by these plants plays the main role in determining the efficiency areas of DME or methanol synthesis plants. There is an electricity cost at which the methanol and DME synthesis plants are equally cost-effective for various given IRR values. This is indicated by the equality of prices of energetically equivalent amounts of DME and methanol, which provide (given a set price of electricity) the required value of IRR. A change in IRR at the points of equal economic viability with a change in electricity price is explained by different ratios of the SLF production to electricity for the considered MPPs. Figure 2 shows the curve of equal cost-effectiveness of the methanol and DME synthesis plants. It is worthwhile to note that the production of dimethyl ether at the modular plant will be more preferable in the off-grid power systems where it is planned to construct such plants because virtually all the electricity produced from the combined DME and electricity production plant is used for auxiliaries.

![Figure 2. The curve of equal economic efficiency of the methanol and DME synthesis plants.](image)

Acknowledgements

The research was carried out under State Assignment, Project 17.1.1 (reg. no. AAAA-A17-117030310433-6) of the Fundamental Research of Siberian Branch of the Russian Academy of Sciences.

References

[1] Schmitz N, Burger J et al 2016 Fuel 185 67-72
[2] Lee M C, Seo S B, Chung J H, Joo Y J and Ah D H 2008 Fuel 87 2162-2167
[3] Tyurina E, Mednikov A, Suchko S 2018 E3S Web of Conferences 69 02008
[4] Huang Z, Qiao X, Zhang W, Wu J, Zhang J 2009 Frontiers of Energy and Power Engineering in China 3 99-108