Mathematical Modeling and Optimization of Gaseous Fuel Processing as a Basic Technology for Long-distance Energy Transportation: The Use of Methanol and Dimethyl Ether as Energy Carriers

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Abstract. The paper presents the results of studies on the perspective technologies of natural gas conversion to synthetic liquid fuel (SLF) at energy-technology installations for combined production of SLF and electricity based on their detailed mathematical models. The technologies of the long-distance transport of energy of natural gas from large fields to final consumers are compared in terms of their efficiency.

1. Introduction
The Asian regions of Russia concentrate sizable energy resources which allow both domestic demands to be met and their considerable volumes to be exported. However, the long distances between the regions with the reserves of energy resources and potential centers of their consumption, primarily in NEA countries essentially increase transportation expenses. This is particularly topical for capital-intensive pipeline transport of natural gas due to shift of its production to hardly accessible areas. These expenses can be reduced to a great extent by natural gas conversion to synthetic liquid fuel.

The pipeline transport of liquid is known to require much lower capital investments and operating costs for pumping than that of natural gas with the same mass of pumped media. It is obvious that the longer the distance to transport an energy carrier, the higher the economic benefit of the SLF transport option in comparison with the natural gas transport. If this benefit exceeds additional expenses for SLF production, the relative total economic efficiency of gas conversion to SLF and its subsequent pipeline transport will be positive.

Methanol production (CH₃OH) from synthesis gas produced in turn from natural gas, is a most promising technology among those of large-scale production of different SLFs. This is associated with high yield and selectivity of the catalytic process of methanol synthesis and also with possible use of methanol as an environmentally clean motor fuel and fuel for boilers and furnaces. However, along with advantages

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methanol as a fuel is characterized by the shortcomings such as toxicity and low heat of combustion (about 21,000 kJ/kg).

At present great interest has been demonstrated in the world to the new energy carrier – dimethyl ether (DME) [1]. At the indoor temperature dimethyl ether is gas, and even at a small pressure (5-8 atmospheres) it is easily liquefied and placed into fuel tanks. In addition to the known advantages of synthetic fuels synthesized from natural gas (absence of aromatic hydrocarbons, sulfur and complete combustion) the dimethyl ether is characterized by the high cetane number (55-60 instead of 40-55 for oil diesel fuel) and also by absence of soot and nitrogen oxides in exhaust gases, which is particularly important for large cities, i.e. it completely adequate to the strict international standards EURO – 4 [2]. In the recent years this fact has given rise to intensive development of production technologies for dimethyl ether (CH₃OCH₃) that is not toxic and has higher heat of combustion (about 29,000 kJ/kg) than methanol. An appreciable progress is achieved in designing a double-stage process of DME production from synthesis gas: methane conversion to synthesis gas (a mixture of carbon oxides and hydrogen) and catalytic synthesis of DME from synthesis gas [4].

It should be noted that production of methanol and dimethyl ether is accompanied by release of large amounts of heat and formation of combustible blast gases. Combined production of SLF and electric power at one energy-technology installation (ETI) is an effective way of utilizing this “energy waste”. The works on modeling ETIs for methanol synthesis and their technical and economic analysis have been conducted at Energy Systems Institute in Irkutsk for a rather long time to come [5-9]. Mathematical models for individual blocks of ETI on coal and natural gas and installation as a whole were constructed. The technical and economic studies performed enabled the calculation of optimal schemes and parameters, on the one hand and the determination of conditions at which ETIs become economically efficient, on the other hand.

In context of the mentioned interest to DME it is pressing to model and investigate ETIs for DME synthesis and to compare their technical and economic characteristics with the corresponding characteristics of ETIs for methanol synthesis and also the costs of DME and methanol transportation.

2. Modeling of ETIs for methanol and DME synthesis

Since in any case DME production passes through the methanol formation stage [5-9], all the suggested technologies of DME synthesis from natural gas are in general an extension of methanol production and comprises some common stages: the stage of natural gas conversion to synthesis gas, the stage of catalytic conversion of synthesis gas to a mixture of methanol and DME, the stage of methanol and DME separation. Therefore, the flow chart of ETI for DME synthesis and electricity production was taken similar to that of ETI for methanol synthesis [5-9]. The installation consists of the following blocks: natural gas conversion, DME synthesis and energy. As distinct from ETI for methanol synthesis, whose simplified flow chart is given in Figure 1.

The conversion block of the installations is designed for natural gas conversion by steam-oxygen blast, cooling and cleaning of conversion products. Live steam and low-pressure steam are generated in the block and supplied to the energy block for electricity production. In the SLF synthesis block the process of catalytic SLF synthesis and generation of low-pressure steam (at the installation of methanol synthesis) coming to the energy block take place. Since the process of DME synthesis from synthesis gas passes through the methanol formation stage and there is residual methanol (4-6% of the volume depending on the synthesis process conditions) at the reactor outlet, it can be used after separation as a desired product or returned to the cycle, which increases a total yield of dimethyl ether. The work studies the latter alternative. The block has three successive synthesis stages with the different number of reactors operating in parallel at each stage. The energy block is intended for combustion of blast gas supplied from the synthesis block, cooling of combustion products and electricity generation by gas and steam turbines.
The studied installations are complex technical systems with a great number of different components connected by diverse technological links. The technical and economic studies on ETI were carried out by the constructed effective mathematical models of installations including both the energy and technology parts. This requires construction of a coordinated system of mathematical models of technological and energy components and subsystems of the installation and solution to the problem of large dimension of the flow charts of ETI when modeling the elements, calculating the schemes and performing technical and economic studies [5-9].

The mathematical model of the natural gas conversion block comprises models of reaction chambers of the converter, radiation and convection heat exchangers, where the conversion products are cooled by water or steam, systems of synthesis gas cleaning. The mathematical model of the SLF synthesis block includes models of synthesis gas compressors, catalytic reactors, regenerative gas-to-gas heat exchangers and refrigerators-condensers. The mathematical model of the energy block includes models of expansion and main gas turbines, air compressor, combustion chamber of the blast gas, steam turbine and waste heat boiler. The applied models are described in detail in [6].

![Flow charts of ETI for dimethyl ether synthesis](image_url)

**Figure 1. Flow charts of ETI for dimethyl ether synthesis:**
a – gas flows, b – air flows, c – feed water flows, d – low-pressure steam flows, e – high-pressure steam flows, f – methanol recirculation, I – block of natural gas conversion, II – block of SLF synthesis, III – energy block; 1 – fuel preparation system, 2 – air separation system, 3 – converter, 4 – system of conversion products cooling, 5 – system of conversion products cleaning, 6 – synthesis gas compressor, 7 – regenerative gas-to-gas heat exchanger, 8 – catalytic synthesis reactors, 9 – refrigerator-condenser, 10 – SLF separator, 11 – expansion turbine, 12 – blast gas combustion chamber, 13 – gas turbine, 14 – air compressor, 15 – waste heat boiler, 16 – steam turbine, 17 – steam turbine condenser, 18 – block of water, methanol and DME separation.
As a result of calculations on the models of ETI the following technical and economic indices were obtained: SLF and electricity production (at the given natural gas consumption), ETI efficiency, capacities of auxiliary power supply, sizes of heating surfaces of heat exchangers, capital investments in particular blocks and the installation as a whole, etc.

Note that in contrast to methanol synthesis the publications devoted to technologies of catalytic DME synthesis from synthesis gas do not present equations of the chemical kinetics of these processes, but indicate only their high selectivity and yield. Conditions of the thermodynamic equilibrium remain in this case virtually the only base for evaluation of synthesis processes. It is precisely such an approach that is applied to the analysis of DME synthesis in [10]. Its use in mathematical modeling of catalytic synthesis processes at the pre-design stages of investigation is feasible in view of the fact that the cost of synthesis reactors makes up only several per cent of the total cost of ETI and the error due to simplified description of processes will not result in essential errors in technical and economic characteristics of ETI. This error is comparable with errors caused by uncertainty of economic information.

3. Study on ETIs for methanol and DME synthesis
Analysis of the flow charts of ETIs shows that the relation between production of methanol or DME and electricity has the greatest effect on the cost of all ETI blocks, its energy efficiency and technical/economic characteristics. Therefore, it is necessary to consider different values of this relation and to determine their associated technical and economic characteristics. The relation depends upon the following key parameters: consumption of steam and oxygen for blast to natural gas converters, which determines a composition of synthesis gas, and the number of reactors placed in parallel at stages of the synthesis block, which in turn determines an extent of synthesis gas conversion to methanol or DME.

Table 1 presents basic initial data applied to calculations of the flow charts of ETIs for synthesis of methanol and DME and determination of their technical and economic characteristics [5-9]. All variants were calculated for the same natural gas consumption of 2.2 billion m³ per year (2.5 million tce/year). The studies on ETI for methanol synthesis were carried out to consider variants with different values of the indicated parameters. By virtue of the simplified description of processes going on in the reactors ETI for DME synthesis was studied only in terms of the impact of oxygen and steam supply to the converter on the relation between production of DME and electric power. Capital investments were determined on the assumption that the number of reactors for DME synthesis at the stages was equal to the number of reactors at the stages of ETI for methanol synthesis (Table 2).

The optimal variant of ETI for DME production is characterized by much lower electricity generation that is used mostly for power supply of the installation itself. This is caused by first, lower heat release at DME synthesis; second, practically full use of CO in the synthesis reactors for DME production. In ETI for methanol synthesis considerable volumes of CO are fed after synthesis to the combustion chamber of the gas turbine.

Table 3 presents final technical and economic characteristics of the technologies compared. As is seen, methanol production is characterized by higher thermal efficiency of SLF synthesis [5]. ETI for DME synthesis has lower capital investments owing to the smaller volume of electric power generation and correspondingly lower capital investment in the energy block. Note that DME production in energy equivalent is much larger than methanol production from the same quantity of synthesis gas.
Table 1. Initial data for calculation of ETI for methanol and DME synthesis

| Parameters, units                                                                 | Values          |
|----------------------------------------------------------------------------------|-----------------|
| Pressure and temperature of conversion process, MPa, K                            | 2, 1373         |
| Pressure of synthesis process, MPa                                               | 8               |
| Gas pressure and temperature at gas turbine inlet, MPa, K                         | 0.96, 1373      |
| Gas at gas turbine inlet, MPa                                                    | 0.96            |
| Specific cost of:                                                                 |
| catalyst, US$/kg                                                               | 7.5             |
| gas turbine, US$/kW                                                            | 600.0           |
| syngas compressor, US$/kW                                                       | 180.0           |
| air compressor, US$/kW                                                          | 120.0           |
| oxygen production, thousand US$//(kg/s)                                          | 200.0           |
| heating surfaces made of low alloy steel, US$/m²                               | 1700.0          |
| heating surfaces made of carbon steel, US$/m²                                  | 1150.0          |
| vessels for conversion block, thousand US$/m                                   | 40.0            |
| vessels for synthesis block, thousand US$/m                                    | 160.0           |
| channels for service water supply system, thousand US$/(t/h)                     | 100.0           |
| coolers for service water supply system, thousand US$/MW                        | 50.0            |
| Specific electricity consumption for oxygen production, kWh/kg                  | 0.3             |
| Share of costs for:                                                              |
| construction and erection works in cost of conversion block equipment           | 0.9             |
| construction and erection works in cost of synthesis block equipment            | 0.6             |
| construction and erection works in cost of energy block equipment               | 1.0             |
| routine maintenances, overhauls, %                                              | 3.5             |
| Share of depreciation charges,                                                  | 0.2             |
| Operating costs, %                                                              | 3.5             |
| Depreciation charges, %                                                         | 4.5             |
| Interest rate of deposit, %                                                     | 7.0             |
| Interest rate of credit, %                                                      | 8.0             |
| Service life of installation, years                                             | 30.0            |
| Period of installation construction, years                                       | 5.0             |
| Number of hours of installed capacity usage per year, hours                      | 7000            |
Table 2. Calculation results of optimal variants of ETI for methanol or DME synthesis and electric power generation

| Parameters, units | ETI for synthesis of | Methanol | DME |
|-------------------|----------------------|----------|-----|
| Specific oxygen consumption for natural gas conversion, kg/kg of fuel | 1.24 |
| Specific steam consumption for natural gas conversion, kg/kg of fuel | 0 |
| Output of conversion products, (kg/s): | | |
| Hydrogen | 12.9 |
| Carbon monoxide | 94.0 |
| Carbon dioxide | 8.9 |
| Steam | 14.4 |
| Methane | 1.5 |
| Production of methyl alcohol or DME from separators, kg/s: | | |
| Stage 1 of synthesis | 35.5 | 42.9 |
| Stage 2 of synthesis | 25.0 | 17.5 |
| Stage 3 of synthesis | 16.3 | 6.8 |
| Mass-to-weight flow rates of blast gases at stage 3 of synthesis block block, kg/s: | | |
| Hydrogen | 3.16 | 1.13 |
| Carbon monoxide | 26.3 | 0.2 |
| Carbon dioxide | 9.13 | 21.6 |
| Steam | 0.05 | 18 |
| Methanol | 0.41 | 0.04 |
| Methane | 1.5 | 1.5 |
| Live steam flow rate at steam turbine inlet, kg/s | 174 | 120 |
| Steam flow rate from high pressure evaporators at steam turbine inlet, kg/s | 146 | 48 |
| Capacity, MW: | | |
| Steam turbine | 332 | 180 |
| Gas turbine | 164 | 75 |
| Expansion turbine | 8.6 | 2.8 |
| Capacity for auxiliary power supply, MW: | | |
| Including capacity of compressors: | | |
| Oxygen | 28.3 | 28.3 |
| Synthesis gas | 43.4 | 54.5 |
| Useful electric capacity of installation, MW | 320 | 60 |
Table 3. Basic technical and economic characteristics of ETI for methanol or DME synthesis and electric power production

| Characteristics                                           | ETI for synthesis of |          |          |
|-----------------------------------------------------------|----------------------|----------|----------|
|                                                           | methanol             | DME      |          |
| Annual consumption of natural fuel, million m³            | 2200                 |          |          |
| Annual consumption of standard fuel, thousand tce        | 2500                 |          |          |
| Annual production of methanol or DME in standard fuel equivalent, thousand tce | 1400 1670 |          |          |
| Annual production of methanol or DME, thousand t           | 1900 1700 |          |          |
| Annual supply of electric power, million kWh             | 2200 400 |          |          |
| Investments in ETI, million dol.                          | 1520 1380 |          |          |
| Thermal efficiency of methanol or DME production, %       | 75.2 70.3 |          |          |

Comparison of installations by the complex economic index – the internal rate of return on capital (IRR) [14] – revealed that the disbursing price of electricity produced by these installations is essential to determine the efficiency regions of ETI for methanol or DME synthesis. The studies showed that for each IRR value there exists such a cost of electricity, at which ETIs for methanol and DME synthesis are equally economical, i.e. the prices of energy-equivalent amounts of DME and methanol, at which the required IRR value is provided (considering the set electricity price), are equal. Variation of IRR at “the point of equal economic efficiency” at the change of electricity price is due to different relations between the SLF and electricity production for the considered ETIs. As an example Table 4 presents (at the same electricity price) the relation between the set IRR values and the associated SLF prices. As is seen from the Table, at IRR somewhat larger than 18% the price of methanol and DME coincides. Figure 2 presents a curve of equal economic efficiency of ETI for methanol and DME synthesis and also zones of economic efficiency of the indicated installations.

Table 4. Prices of methanol and DME at different IRR levels (price of supplied electricity – 5 cent./tce), dol./tce

| IRR, % | ETI for synthesis of methanol |          |          |
|--------|-------------------------------|----------|----------|
|        |                               | DME      |          |
| 12     | 160                           | 164      |          |
| 15     | 174                           | 178      |          |
| 18     | 190                           | 194      |          |
| 21     | 206                           | 209      |          |
Figure 2. IRR characterizing points of equal economic efficiency of ETI for methanol and DME synthesis as a function of electricity supplied: 1 – the efficiency zone of ETI for DME synthesis, 2 – the efficiency zone of ETI for methanol synthesis

It should be underlined that the technology of DME production at ETI will be preferable, if it is impossible to sell excessive electricity in a power systems, where construction of ETI is planned, since virtually all the electric power generated by the installation for DME synthesis is used for its own requirements.

4. Long-distance transport of natural gas energy based on its conversion to SLF

Evaluation of the economic efficiency of SLF production from natural gas will be incomplete without considering the effect from decreasing the costs at a transition from the pipeline transport of natural gas to SLF.

It was evaluated by the mathematical models of pipeline systems comprising detailed models of linear parts, compressor and pumping stations. Capacity and expenses for unit energy transport for gas and SLF pipelines were optimized at stage 1 of studies. Optimization was performed using these models for different diameters of pipelines depending on the specific cost of their linear parts. The optimal capacities of pipelines were determined by minimizing the cost of transporting an energy unit at the given level of internal rate of return on capital [15, 16]. As a result the optimal capacities of pipelines of natural gas, methanol and dimethyl ether were calculated. Here depending on the specific investments in linear parts and standard sizes specific costs for natural gas transport per 1000 km are $18-45/tce for methanol transport – $9-18/tce for DME pipelines – $8-14/tce.

Then the comparative studies on the economic efficiency of different technologies for natural gas energy transport (Figure 3 a, b) were carried out and are presented below.

1. Natural gas transport by pipelines (GPL1420).
2. Natural gas conversion to methanol and its transport by the methanol pipeline (ETI\textsubscript{meth} + pipeline).
3. Natural gas conversion to DME and its transport by the DME pipeline (ETI\textsubscript{DME} + pipeline).
It was an optimization problem with IRR maximization at the given energy cost [14]. A competitive cost of energy resources for final consumers was taken by the expert judgements substantiated in [15, 16] to be $127-175/tce for natural gas and $145-200/tce for SLF. The natural gas price in situ was taken equal to $30/thousand m³, the price of electricity produced by ETI makes up 3.5 cent./kWh. Table 5 illustrates technical and economic indices of pipelines. The initial data on ETI for SLF production are borrowed from Table 3.

**Table 5. Assumed technical and economic indices of pipelines**

| Parameter, units | Diameter of pipeline of | 1420 mm | 1220 mm |
|------------------|-------------------------|---------|---------|
| 1. Nominal pressure, MPa | gas | 7.4 | 5.4 |
| 2. Base specific cost of linear part, mln. dol./km | methanol or (DME) | 2.3 | 1.3 (1.43)^2 |
| 3. Fixed component of investment in pumping station, mln. dol. | | 21 | 10 |
| 4. Variable component of investment in pumping station, dol./kW | | 300 | 600 |
| 5. Specific fuel consumption by driving gas turbines of compressor stations, gce/kWh | | 384 | - |
| 6. Price of electricity for electric drive of pumping stations, cent./kWh | | - | 5 |
| 7. Calculated low calorific value of natural gas or SLF, MJ/m³, MJ/kg | | 33.5 | 21 (29)^3 |
| 8. Utilization of nominal capacity per year, hours | | | 8000 |
| 9. Operating costs, % of investment | | | 3.5 |
| 10. Depreciation charges, % of investment | | | 6 |

^2 In brackets is the cost of a linear part of methanol pipelines with a 10% increase in capital investment due to additional measures on environmental security of methanol transport.

^3 In brackets is the low calorific value of DME.
The plots show that the technology of DME production from natural gas and its subsequent transport is advantageous over natural gas transport even at distances 2-2.5 thousand km and over the technology of methanol production and transport in the whole range of distances considered. The technology of methanol production from natural gas and its pipeline transport is highly economically efficient in comparison with that of natural gas transport by the 1420 mm pipeline starting with distances from 3500-4200 km. The studies performed allow the conclusion that comparison of the technologies of large-scale natural gas energy transport from the Asian regions of Russia to remote consumers reveals an essential economic advantage of natural gas conversion to dimethyl ether with its further transport by DME pipelines.

It should be underlined that the options of energy transport essentially differ in the volumes of primary energy consumed. For example, in the option with natural gas transport by the 1420 mm pipeline the yearly natural gas use totals 34 billion m³ (39 million tce). For methanol production from natural gas by ETI for subsequent transport of 100 million t (72 million tce) gas consumption makes up about 110 billion m³ per year (127 million tce). Electricity generation in this case will be some 112 billion kWh. Gas consumption to produce 100 million t of DME (99 million tce) at ETI equals 130 billion m³ per year (150 million tce) with generation of 25 billion kWh of electricity.

5. Conclusion
Comparison of the described technologies of SLF synthesis shows that ETI for DME and methanol synthesis have their own regions of efficiency that are determined by the price of electricity produced by ETI. However, the higher consumer qualities of DME and lower expenses for its transportation make the technology of the single-stage production from synthesis gas more promising.

The technologies of natural gas conversion to SLF with subsequent transport to final consumers become more profitable with the growing distances of natural gas energy transport.

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