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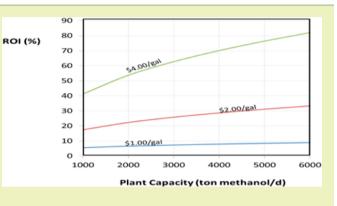
Process Design and Integration of Shale Gas to Methanol

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ABSTRACT: The substantial discoveries of shale gas present many opportunities for the chemical, petrochemical, and fuel industries. As in conventional natural gas, shale gas contains primarily methane, but some formations contain significant amounts of higher molecular weight hydrocarbons and inorganic gases such as nitrogen and carbon dioxide. These differences present several technical challenges to incorporating shale gas with the current infrastructure designed to be used with natural gas. This paper is aimed at process synthesis, analysis, and integration of the production of methanol from shale gas. The composition of the shale gas feedstock is assumed to come from the Barnett Shale play located near Fort Worth, Texas, which is currently the most active shale gas play



in the United States. Process simulation using ASPEN Plus along with published data were used to construct a base-case scenario. Key performance indicators were assessed. These include overall process targets for mass and energy and economic performance. A sensitivity analysis is carried out to assess the impact of the methanol selling price and shale gas price on the profitability of the process. Energy integration including process cogeneration was carried out to enhance the sustainability and profitability of the process. Finally, a techno-economic analysis was carried out to estimate the price differential for shale gas at the wellhead compared to pipeline quality natural gas.

KEYWORDS: Shale gas, Natural gas, Methanol, Process integration, Process simulation, Techno-economic analysis, Barnett Shale

INTRODUCTION

In order to meet the energy demands of the twenty-first century, engineers and scientists are working to develop new methods of discovering, extracting, and refining fossil fuels including oil, coal, and natural gas. While the development of alternative energy technologies continues and the use of renewable energy sources increases, fossil fuels still fulfill the majority of the United States' energy needs, which is approximately 85% total, with natural gas supplying about 22% of this total.¹

As the demand for natural gas continues to rise, new sources and techniques for extracting natural gas are being developed. Unconventional production, which includes but is not limited to shale gas production, now accounts for 46% of the total United States production of natural gas.¹ Shale gas production and infrastructure in the United States have been growing consistently over the past decade and is projected to increase over the next two decades to become the primary source of natural gas produced in the United States.² Shale gas includes natural gas sources from low-permeability shale, a sedimentary rock that consists primarily of consolidated clay-sized particles. Breakthroughs in modern drilling technology (hydraulic fracturing or "fracking") have overcome the low permeability of shale and have made it possible to increase gas flow from the shale formation and make development of shale reservoirs economical. Drilling of shale gas wells includes both traditional vertical wells as well as horizontal wells. Horizontal well drilling has become an increasingly utilized technique because it provides exposure to a greater volume of a formation; a single well pad with horizontal wells can access the same reservoir volume as 16 vertical wells.¹ As a result, fewer drill pads are necessary, which also reduces the infrastructure necessary to develop a well. While helping to optimize product recovery and profit, these techniques can also help to reduce the overall environmental impact of gas recovery and production.

Similar to natural gas, the largest fraction of shale gas consists of methane. However, some shale gas formations contain significant amounts of higher molecular weight hydrocarbons, including ethane and propane, as well as other inorganic gases such as nitrogen and carbon dioxide. Table 1 shows typical compositions of shale gas from different reservoirs.

Compounds in shale gas may not be present in natural gas or may be present only in negligible amounts. These differences present several technical challenges to incorporating the use of shale gas with the current infrastructure designed to be used with conventional natural gas. Each shale gas basin presents many opportunities to develop novel chemical processes that

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Table 1. Average Shale Gas Compositions from Wells³

	•	-	-		
reservoir	C1	C2	C3	CO ₂	N_2
Barnett	86.8	6.7	2.0	1.7	2.9
Marcellus	85.2	11.3	2.9	0.4	0.3
Fayetteville	97.3	1.0	0.0	1.0	0.7
New Albany	89.9	1.1	1.1	7.9	0.0
Antrim	62.0	4.2	1.1	3.8	29.0
Haynesville	95.0	0.1	0.0	4.8	0.1

optimize its composition in order to more efficiently and profitably produce valuable chemical products.

For shale gas to be transported via the existing natural gas pipeline infrastructure, treatment is needed. Although no national standards exist, each pipeline has strict specifications for heat content, removal of particulate matter, and maximum concentrations of contaminants such as nitrogen, carbon dioxide, and hydrogen sulfide, and natural gas liquids. Typical gas treatment may involve three main steps: removal of impurities, dehydration, and separation into light and heavy fractions. In order to prepare the crude gas for processing, first acid-forming components such as carbon dioxide and hydrogen sulfide must be removed. Dehydration is central to the purification process in order to prevent condensation inside pipelines during transport. Similarly, some pipeline standards do not allow for high nitrogen content, so nitrogen is typically removed via a cryogenic separation process and discharged to the atmosphere. Additionally, drilling process water must be treated due to soluble contaminants from the gas and particulate matter (i.e., dirt and sand) that infiltrate the water during the drilling process. For example, removal of impurities, dehydration, and separation into light and heavy fractions is needed.

Numerous products can be made from shale gas. A particularly important chemical is methanol because it plays a crucial role as a reactant in the manufacture of many other basic chemical compounds such as formaldehyde, acetic acid, methyl halides, methyl tert-butyl ether, dimethyl terephthalate, methyl-amines, methyl methacrulate, and industrial solvents.^{4,5} Methanol can also be used as a fuel or a fuel additive. Methanol manufacture can use a combination of feedstocks. While natural gas and shale gas are expected to be the primary feedstock for methanol plants in the United States, carbon dioxide can be added to the raw materials to enhance the efficiency of natural gas utilization and to provide an effective method for carbon recycle carbon dioxide.^{6,7}

The purpose of this paper is to develop a process synthesis, simulation, and integration of a shale gas-to-methanol plant. Computer-aided simulation along with literature data are used to develop a base case scenario. Techno-economic analysis is undertaken to assess the profitability of the process under current market conditions. A sensitivity analysis is also carried out to examine the impact of market variability on the process economics.

PROBLEM STATEMENT

Given shale gas from a certain reservoir, it is desired to synthesis, simulate, and integrate a methanol production plant and to carry out techno-economic analysis to answer the following questions: (1) What is the necessary pretreatment of shale gas? (2) How does the process flowsheet look like? (3) What are the key mass and energy performance metrics? (4) What are the economic criteria of the process? How do they vary under market variability? (5) What is the cost differential between shale gas and natural gas to perform the same task of producing methanol?

A base case of a 5000 ton per day methanol plant is used. An on-stream factor of 0.904 (corresponding to 330 operating days or 7920 operating hours per year) is used. The shale gas is taken to represent values from gas produced from the Barnett Shale play, located in northeast Texas near the Fort Worth area.³ The area was first developed in the 1980s and was nicknamed the "Grandfather Shale" because it served as the development ground for the modern techniques that made shale gas production economical in the United States. It continues to be the most active shale gas play in the United States. Values for composition of various wells from the Barnett Shale are shown in Table 2. These data show the wide

Table 2. Barnett Sha	le Gas Composition [°]
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well	C1	C2	C3	CO ₂	N_2
1	80.3	8.1	2.3	1.4	7.9
2	81.2	11.8	5.2	0.3	1.5
3	91.8	4.4	0.4	2.3	1.1
4	93.7	2.6	0.0	2.7	1.0
average	86.8	6.7	2.0	1.7	2.9

variability of possible chemical compositions of shale gas formations. While some areas of the Barnett Shale play are fairly consistent with conventional natural gas sources, others contain much higher concentrations of hydrocarbons, carbon dioxide and nitrogen. Data from Well 1 were used in the simulation of the base case.

PROCESS DESCRIPTION

Before the shale gas feedstock can be sent via a pipeline to the methanol plant, it must first undergo several preprocessing steps in order to remove contaminants that are limited by pipeline standards. As shown in Figure 1, the shale gas is first sent through an acid gas removal unit followed by a dehydration unit and a nitrogen gas separation unit. The nitrogen removal unit (Figure 2) is typically a membrane separation process (gas permeation) that produces a reduced nitrogen natural gas stream and a nitrogen-rich stream that can be used as fuel. Recycling is used to enhance the recovery of nitrogen and fuel gas. The nitrogen-reduced gas is cooled via a heat recovery exchanger and a feed cooler and sent to a series of cryogenic distillation columns in order to recover the natural gas liquids (NGLs). The first cryogenic column is the demethanizer and is designed to remove methane from the higher boiling hydrocarbons using 15 theoretical stages. The second cryogenic column is the de-ethanizer and separates ethane from higher boiling hydrocarbons using 23 theoretical stages. The recovered NGL from the shale gas is purified in this step to be sold for a profit.

Figure 3 is a schematic representation of the process flowsheet. Methanol is typically produced on an industrial scale using a catalytic reaction of synthesis gas at high pressure. In order to produce methanol, first syngas must be generated. The production of synthesis gas (syngas) may be achieved via partial oxidation, steam reforming, or autothermal reforming. There are various trade-offs for cost, energy, H_2 :CO ratio, water consumption, and environmental impact. Optimization and selection among the three syngas generation processes requires a much more complex analysis that is beyond the scope of this work. For more information on these design considerations, the reader is referred to Noureldin et al.⁷ In this paper, partial oxidation was selected. For partial oxidation, methane is reacted with oxygen from air according to the following exothermic reaction

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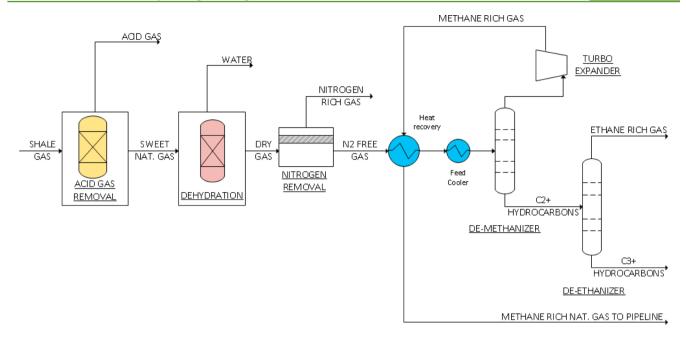
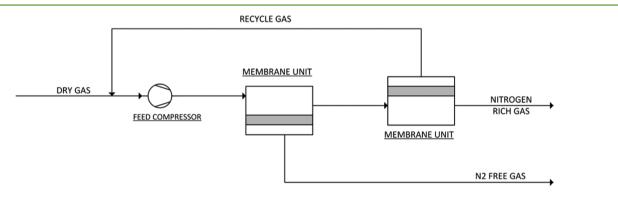


Figure 1. General gas processing flow diagram.



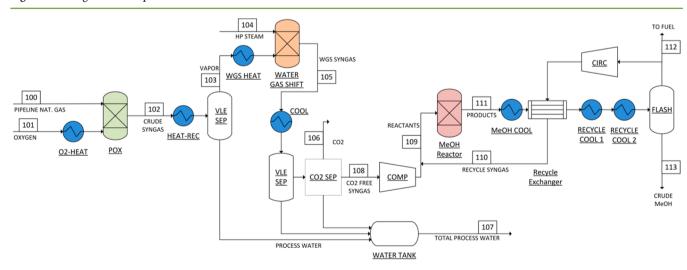
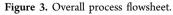


Figure 2. Nitrogen removal process.



$$CH_4 + 1/2O_2 \leftrightarrow CO + 2H_2 \quad \Delta Hr = -36 \text{ kJ/mol}$$
 (1)

Oxygen present in excess or insufficient amounts will result in the formation of the byproducts carbon dioxide and coke (solid carbon). In this work, the syngas generation through partial oxidation was modeled using data from Bao et al.⁸ For this analysis, the partial

oxidation process was selected for the simulation of syngas generation because the reaction is exothermic and does not yield excess hydrogen. The maximum yield for synthesis gas generation occurs when the components are present in a stoichiometric ratio of 2:1 (sometimes referred to as metgas⁹). In reality, partial oxidation leads to a CO/H_2 ratio of about 1.8.

Data
Stream
Key
ë
Table

													-					
crude MeOH	113	0.0	2.7	30.8	2.1	0.0	0.0	403.7	12524.5	1.8	0.4	0.7	0.0	55.1	13021.8	415835	113	1096
to fuel	112	5007.9	0.0	19.7	13.2	0.0	0.0	1981.6	55.0	0.0	0.1	0.0	0.0	24.2	7101.7	69119	113	1096
products	111	10015.8	2.7	70.2	28.6	0.0	0.0	4367.0	12634.6	1.8	0.5	0.7	0.0	103.4	27225.3	554072	464	1102
recycled syngas	110	5008.2	0.0	19.7	13.2	0.0	0.0	1981.8	55.0	0.0	0.1	0.0	0.0	24.2	7102.2	69125	248	1102
	109																	
CO ₂ -free syngas	108	30109.3	94.7	50.5	15.3	0.0	0.0	15052.0	0.0	0.0	0.0	0.0	0.0	2.7	45324.5	485374	104	573
	107																	
	106																	
WGS syngas	105	30109.3	145.0	50.6	15.3	0.0	0.0	15053.2	0.0	0.0	0.0	0.0	0.0	1744.4	47117.9	562965	614	573
HP steam	104	0.0	984.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	984.0	17727	481	573
vapor	103	29174.8	95.5	50.6	15.3	0.0	0.0	15987.7	0.0	0.0	0.0	0.0	0.0	809.9	46133.8	545238	104	573
crude syngas	102	29174.8	4749.6	53.3	15.4	0.0	0.0	16108.0	0.0	0.0	0.0	0.0	0.0	948.8	51049.9	638614	2318	363
oxygen	101	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11291.6	0.0	11291.6	361316	79	377
pipeline, nat. gas	100	0.0	0.0	16989.8	15.4	17.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	86.0	17108.3	277297	79	377
		lbmol/h																
component	stream number	hydrogen	water	methane	nitrogen	ethane	propane	carbon monoxide	methanol	butanol	dimethyl-ether	acetone	oxygen	carbon dioxide	total flow	total flow (lb/h)	temperature $(^{\circ}F)$	pressure (psia)

Table 4. Key Economic Results for the Base Case Design

Research Article

item	rate	unit cost	annual cost (\$MM/yr)
shale gas (delivered, pipeline quality)	155.8 MMSCF/d	\$3.50/kSCF (or/MMBtu)	179.95
oxygen	361,394 lb/h	\$0.05/lb	143.11
heating utility	180 MMBtu/h	\$4.00/MMBtu	5.70
cooling utility	1414 MMBtu/h	\$1.94/MMBtu	21.73
power consumption	14,746 kW	\$0.05/kWh	5.84
waste treatment	1140 ton/d	\$0.48/ton	0.18
labor			3.80
methanol sales	5000 ton/d	\$2.00/gal (\$600/ton)	990

In the O₂-Heat exchanger, oxygen gas is heated to 473 K. The heated oxygen and pipeline natural gas (here assumed to be shale gas that has been purified using the process described above and transported to the plant site via pipeline) are fed to the partial oxidation (POX) reactor, where the raw materials react at 19.7 atm in order to form crude synthesis gas comprised of hydrogen gas and carbon monoxide in approximately a 1.8:1 ratio. In the heat-recovery (Heat-Rec) exchanger, the products are cooled to 313 K and pressurized to 39.0 atm. In order to adjust the ratio to the stoichiometric value of 2.0, the gas mixture is sent through a flash column (vapor–liquid equilibrium separator or VLE-SEP) and then to the water–gas shift (WGS) reactor at 573 K where the WGS reaction occurs.

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad \Delta Hr = -41.1 \text{ kJ/mol}$$
 (2)

Next, the products from the WGS reactor are cooled to 313 K and sent to another flash column (VLE-SEP) where the liquid water separates from the syngas. Next, carbon dioxide is removed in the CO_2 SEP unit, and the gas is compressed in the COMP unit to 75 atm and sent to the MEOHRXR reactor where it reacts at 513 K to form methanol vapor. The products from this reaction are then sent through a recycle loop with heat exchangers RECYCLE COOL 1 and RECYCLE COOL 2 and the CIRC compressor in order to maximize conversion of the feedstock. The crude methanol product is separated from the recycle stream in a flash column (FLASH) with the recycle ratio set at 0.5.

Equilibrium for methanol formation is favored by low temperatures and high pressures, so the reactor feed conditions⁵ are typically 50– 100 atm and 503–533 K. The reaction takes place over a CuO/ZnO/ Al₂O₃ catalyst. Methanol synthesis actually occurs as a combination of two reactions in the syngas mixture. The first involves carbon dioxide and hydrogen, and the second involves carbon monoxide and water generated in the system. The overall reaction shows a net exothermal conversion of carbon monoxide and hydrogen gases, the primary components of syngas, to liquid methanol.

$$CO_{(g)} + H_2O_{(g)} \leftrightarrow H_{2(g)} + CO_{2(g)} \quad \Delta H^{298} = -41 \text{ kJ/mol}$$
(3)

$$CO_{2(g)} + 3H_{2(g)} \leftrightarrow CH_3OH_{(1)} + H_2O_{(g)} \quad \Delta H^{298} = -50 \text{ kJ/mol}$$

(4)

$$CO_{(g)} + 2H_{2(g)} \leftrightarrow CH_3OH_{(l)} \quad \Delta H^{298} = -91 \text{ kJ/mol}$$
 (5)

During this process, some side reactions occur that form impurities including dimethyl ether, methyl formate, and butanol, which must be removed during the final purification of the process. The methanol reactor was modeled using a temperature of 513 K and pressure of 75 atm and primary chemical reactions and side reactions using the RGIBBS thermodynamic equilibrium model of ASPEN Plus simulation. In order to perform the analysis, information was gathered from various sources in order to estimate captial cost and operating costs. Cost of utilities, raw materials, and labor were extracted from literature coupled with simulation results .

The shale gas preprocessing cost and profit from NGL separation was estimated from literature values and flow rates from the simulator. The preprocessing cost was then used to determine a price differential between natural gas and shale gas. Once impurities are removed from natural gas feedstocks, the hydrocarbons are separated into light and heavy fractions through cooling and partial condensation in a heat exchanger. Modern plants use cryogenic separation to separate propane and butane, also known as liquefied petroleum gas (LPG). In this process, crude gas is cooled and partially condensed under high pressure in a heat exchanger and then expanded, heated, and sent to a separation column where the bottoms products consist of the C3 plus products and the light hydrocarbons (ethane and methane) are recycled from the top of the column. Ethane is separated in a similar manner as the LPG process but with a lower temperature profile. Autothermal reforming combines the previous two techniques by using the energy generated from partial oxidation of hydrocarbons to drive the endothermic reaction in steam reforming.

RESULTS AND DISCUSSION

The following assumptions¹⁰⁻¹² and data were used in the economic analysis: (1) The fixed capital investment (FCI) was estimated based on the cost of a 5000 ton/day methanol plant¹² (\$MM 1300) and the six-tenths factor rule to be

FCI(in \$MM) = 7.8444

$$\times$$
 (plant capacity in ton methanol/day)^{0.6} (6)

(2) A ten-year linear depreciation scheme was taken with a salvage value of 10% of the FCI. (3) The working capital investment (WCI) was assumed to be 15% of the total capital investment (TCI) where TCI is the sum of FCI and WCI. (4) A tax rate of 30% was used. (5) An on-stream factor of 0.904 (corresponding to 330 operating days or 7920 operating hours per year) is used.

The stream-data results of process simulation are shown in Table 3. These results along with cost estimations were used to generate the economic data shown in Table 4 for the base case design.

A sensitivity analysis was performed to evaluate the ability of the process to withstand changes in feedstock and product values (Figure 4). The return on investment (ROI) is used to evaluate the potential profitability of the process. The ROI is defined as¹¹

$$ROI = \frac{annual after-tax profit}{total capital investment (TCI)}$$
(7)

where

annual after-tax profit

- = (annual revenues annual operating cost
 - depreciation) \times (1 tax rate) + depreciation (8)

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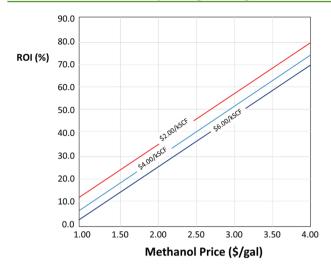
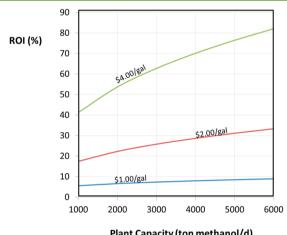


Figure 4. Sensitivity analysis for the ROI of the base case design (5000 ton/d) at various prices of shale gas.

Figure 5 shows the ROI against methanol price ranging from

\$1.00 to \$4.00 per gallon and shale gas price (delivered to the



Plant Capacity (ton methanol/d)

Figure 5. Sensitivity analysis for the ROI vs plant capacity at various prices of methanol (price of shale gas = 3.5/kSCF).

plant at pipeline quality) ranging from \$2.00 to \$6.00 per kSCF. For the economic data listed in Table 4 (methanol price of \$2.00/gal and shale gas cost of \$3.50/1000 MMBtu), a 31% ROI is achieved, which is attractive enough. More attractive ROIs are attained for lower gas prices and higher methanol-selling prices.

The effect of plant capacity is another important sensitivity factor. Figures 5 and 6 illustrate the impact of plant capacity on the ROI for different prices of methanol (Figure 5) and shale gas (Figure 6). Typically, a minimum ROI of 15% is required for most new process. As such, if the price of methanol drops to \$1.00/gal, the process becomes economically unattractive regardless of the plant capacity and the shale gas price (within the studied ranges).

Because shale gas must undergo pretreatment prior to being fed into the natural gas pipelines, it is useful to estimate the price differential compared to natural gas. Analysis of the inlet gas stream was used to estimate the preprocessing cost for shale gas. The primary cost factors included were acid gas removal and nitrogen gas removal. Additionally, some of the total cost is

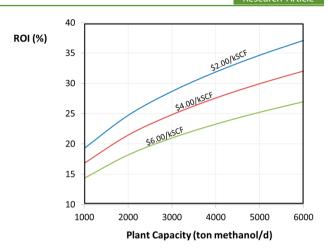


Figure 6. Sensitivity analysis for the ROI vs plant capacity at various prices of shale gas (price of methanol = \$2.0/gal).

offset through separation of the natural gas liquids (NGLs) ethane and propane. Process simulation and cost estimation were carried out for the pretreatment and recovery systems. The final cost was then used to determine a price differential between shale gas from the wellhead in comparison with pipeline-quality natural gas. Key results are shown in Tables 5 and 6. As shown in Table 6, the estimated price differential for shale gas at the wellhead is \$0.73/kSCF compared to pipeline quality natural gas.

Table 5. Preprocessing Cost Estimation

	flow rate (lb mol/h)	total annualized cost (MM/yr)
acid gas removal	23148	25.95
N ₂ removal	23148	90.45
C2 credit	1875	35.85
C3 credit	532	42.92
total		37.63

Table 6. Shale Gas/Natural Gas Price Differential

	unit cost (\$/kSCF)
natural gas	3.50
shale gas	2.77
price differential	0.73

Energy Integration. The process has several heating and cooling duties. The O2-Heat exchanger takes the inlet stream OXYGEN and heats it to 473 K before entering the POX reactor. The heat-recovery (Heat-Rec) exchanger cools the syngas mixture stream SG1 from the POX reactor down to 313 K and compresses the mixture to 39.0 atm. Condensed liquids are separated from the gas stream in the flash column, and then the gas stream is heated again in the WGS-Heat exchanger to 573 K before entering the WGS reactor. The products from this reactor are then sent to the Cool exchanger where they are again cooled to 313 K. Unit MeOH Cool takes the products from the methanol reactor and cools them to 423 K and expands them to 80 atm. Units Recycle Cool 1 and Recycle Cool 2 continue to step down the temperature and pressure to 333 K and 76.3 atm and then 318 K and 74.6 atm before the crude methanol product is separated from the recycle stream in a final flash column.

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Table 7. Heat Exchanger Data

heat exchanger tag	description	supply temperature (K)	target temperature (K)	heat duty (kW)
O ₂ -Heat	oxygen heater before reforming	299	473	7614
WGS-Heat	heater before water-gas shift reaction	313	573	45,129
Heat-Rec	cooler for syngas leaving the reformer	1544	313	-283,206
Cool	cooler after water-gas shift reactor	597	313	-51,008
MeOH Cool	cooler after the methanol reactor	513	423	-42,389
Recycle Cool (1 and 2) two co	ooler for crude methanol product before entering the final flash column	420	318	-37,093
	1600			
Т (К)	1500			
	1400			
	1300			
	1200			
	1100			
	1000			
	900			
	800			
	700			
	600			
	500			
	400 -			
	300		_	
	0 50 100 150 200 2	50 300 3	50 400	
	Residual Heat (MW)		um Cooling = 360.95 MW	

Figure 7. Grand composite curve for heat integration of the methanol plant.

The operating cost can be reduced through the use of heat integration and cogeneration. The data for the hot and cold streams are given in Table 7.

Heat integration among the process hot and cold streams is carried out using the thermal pinch analysis. The grand composite curve for the heat integration network is shown in Figure 7. For information on constructing such diagrams, the reader is referred to process integration testbooks.^{11,13} The vertical axis is the average temperature of the hot and cold streams that are separated by a minimum driving force of 10 K. The horizontal axis is the residual heat. As shown in Figure 7, the targets for minimum heating and cooling utilities are reduced to 0 and 1232 MMBtu/h (360.95 MW). The cooling utility can be further reduced and electric power can be produced using cogeneration. Excess heat is extracted from the hot streams to produce steam that is let down through turbines. One method for evaluation cogeneration targeting is based on the use of extractable energy of streams, which corresponds to the enthalpy times energy extraction efficiency times the flow rate of each steam stream associated with a header.¹⁴ Next, composite curves are constructed for the surplus and demand of steam headers. By combining these composite curves a target can be determined for combined heat and power (cogeneration). The details of this approach are described in the literature.¹⁴ Using this method of combined heat and power targeting, the cooling utility is reduced to 620 MMBtu/h, and the cogenerated electric power is 90.54 MW. Because the total power demand of the process is 14.75 MW, the net power generation of the process is 75.79 MW. This corresponds to an annual value of \$30.01 MM/yr. The sensitivity analysis shown in Figure 8, which accounts for the savings due to energy integration, shows a corresponding increase in ROI of approximately 2.5%.

CONCLUSIONS

Process synthesis, simulation, and integration were carried out to establish a basis for the techno-economic analysis of shale gas-to-methanol production. The results of the technoeconomic analysis demonstrate that production of methanol from shale gas would be profitable for a broad range of methanol selling prices and shale gas costs. For instance, a desirable 31% ROI is achieved for a methanol selling price of \$2.00/gal and shale gas price of \$3.50/kSCF. The sensitivity analysis shows that the process operating cost depends primarily on the prices of methanol and shale gas. For a broad range of combinations of shale gas and methanol prices, the process enjoys a favorable ROI. Energy integration corresponds to an increase in ROI of approximately 2.5% for the base case.

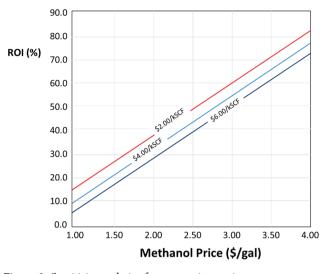


Figure 8. Sensitivity analysis after energy integration.

Further analysis led to a cost estimation for the preprocessing of shale gas required to reach pipeline standards, which is necessary for delivery of the raw material to the proposed plant site. Because shale gas can have a chemical composition much different than natural gas, these preprocessing costs may lead to a price differential between shale gas and conventional gas. In the scenario analyzed for shale gas from the Barnett Shale play, the preprocessing costs were dominated by nitrogen removal, with some of the costs being offset from the sale of natural gas liquids (C2 and C3). However, these preprocessing costs require that the shale gas from the wellhead be sold at a lower price than pipeline-quality natural gas. This case shows a price differential at \$0.73/MMBtu, but other sources of shale gas with fewer impurities would have a narrower price differential.

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Notes

The authors declare no competing financial interest.

REFERENCES

(1) Nash, K. M. Shale Gas Development (Energy Science, Engineering, and Technology); Nova Science Publishers: New York, 2010; p 174.

(2) Goellner, J. F.; Krouskop, P. E. Expanding the shale gas infrastructure. *Chem. Eng. Prog.* **2012**, *108* (8), 49–52.

(3) Bullin, K. A.; Krouskop, P. E. Compositional variety complicates processing plans for US shale gas. *Oil Gas J.* 2009, 107 (10), 50–55.
(4) Hans-Jürgen, A. *Industrial Organic Chemistry*, 5th ed.; Wiley

VCH: Weinheim, Germany, 2010.

(5) Cheng, W. H., Kung, H.H., Eds.; Methanol Production and Use; Marcel Dekker: New York, 1994.

(6) Olah, G. A.; Goeppert, A.; Prakash, G. K. S. *Beyond Oil and Gas: The Methanol Economy*, 2nd ed.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 2009.

(7) Noureldin, M.M. B.; Bao, B.; Elbashir, N. O.; El-Halwagi, M. M. *Process Design and Integration of XTL Plants.* Presented at the 243rd ACS National Meeting, San Diego, March 2012.

(8) Bao, B.; El-Halwagi, M. M.; Elbashir, N. O. Simulation, integration, and economic analysis of gas-to-liquid processes. *Fuel Process. Technol.* **2010**, *91* (7), 703–713.

(9) Olah, G. A.; Goeppert, A.; Czaun, M.; Surya Prakash, G. K. Bireforming of methane from any source with steam and carbon dioxide exclusively to metgas $(CO-2H_2)$ for methanol and hydrocarbon synthesis. *J. Am. Chem. Soc.* **2013**, *135*, 648–650. (10) Peters, M. S.; Timmerhaus, K.D.; West, R.E. *Plant Design and Economics for Chemical Engineers*, 5th ed.; McGraw-Hill: New York, 2003.

(11) El-Halwagi, M. M. Sustainable Design through Process Integration: Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement; Butterworth-Heinemann: Oxford, 2012.

(12) Sider, A. Louisiana Group Plans To Build Largest Methanol Plant in North America. *Hydrocarbon Processing*, March 1, 2013.

(13) Kemp, I. Pinch Analysis and Process Integration: A User Guide on Process Integration for the Efficient Use of Energy, 2nd ed.; Butterworth-Heinemann: Oxford, 2009.

(14) El-Halwagi, M. M.; Harell, D.; Spriggs, H. D. Targeting cogeneration and waste utilization through process integration. *Appl. Energy* **2009**, *86* (6), 880–887.