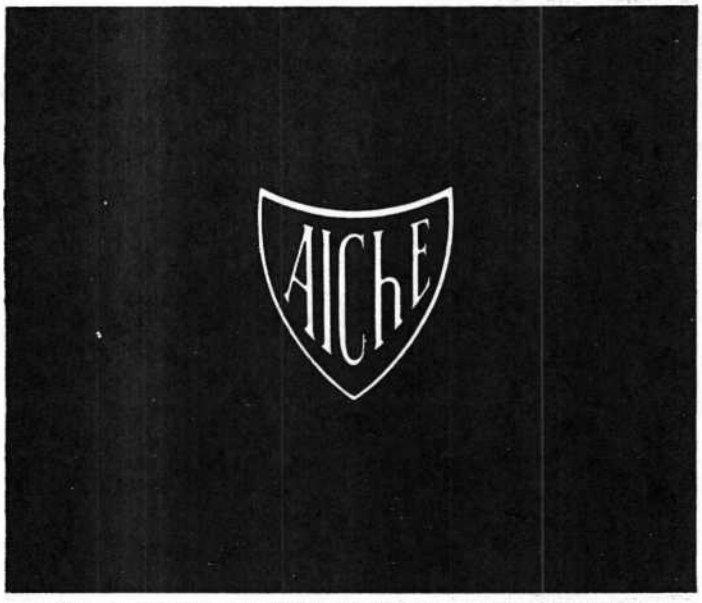

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THE CO-PRODUCTION OF METHANOL AND ELECTRICAL POWER FROM COAL

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The Co-Production of Methanol and Electrical Power from Coal

Methanol produced on site can add flexibility to utility companies in meeting extreme peak load demand.

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This paper describes an investigation with a computer model of a new process to co-produce electrical power and methanol in a coal gasification process. The methanol can be used either as a fuel or a commodity, depending on the utility requirements. Use is made of membrane separators (or pressure swing adsorbers) to eliminate the need for the CO shift reactor and some of the subsequent processing steps used in the normal methanol production route from coal.

Advanced features of flowsheet simulators were used to examine both the feasibility of this process and the possibilities for improving its overall economics. The development of commercially available process simulators provides engineers the capability of evaluating new processes that incorporate different proprietary equipment or a licensed process in a fully integrated arrangement. The simulator, DESIGN II[SM], used in this work provides the option of adding a model to those models already built into the process simulator. This option was used for modeling membrane separators.

BACKGROUND

There is reason to believe that coal gasification will gain renewed interest in the next several years as a means of producing electricity. The Power Plant and Industrial Fuel Use Act requires that neither oil nor natural gas be consumed as the primary energy source in any new electric power plant unless exempted such as in cogeneration facilities. A recent study [*1*] carried out by the Bechtel Group has predicted a short fall in available electrical power nationwide between 1985 and 1990, depending on the actual GNP realized in the US. The 1985 figure was based on a 4.5% GNP and the 1990 figure would require a GNP of only 2.5% which is the figure for a "status quo" economy. Any new power producing facilities created by these demands will very likely be required to be either nuclear or coal fired. Since there are a number of problems with nuclear derived power, the short to medium term prospects would appear to be better for coal.

This is a study of a process designed to reduce the capital cost for the co-production of methanol along with electrical power from a coal gasification plant. Utility companies are confronted with a wide variation of electrical power demand throughout the year. A power plant designed for the peak demand is only partially utilized the majority of the time. Alternatively, utility companies often meet their peak loads by burning relatively high cost premium fuels. If methanol is produced and stored during off-peak periods it can be used as a less expensive fuel during peak periods, thus helping to stabilize cost for peak demand.

In addition to this, there are a number of other reasons for examining the feasibility of co-producing methanol with a coal power production facility: 1) methanol can be stored in less volume per unit of energy and more cheaply than gas; 2) methanol is a clean burning fuel; 3) methanol can be used in a standard gas turbine (with minor burner modifications); 4) the technology for methanol production is established. In addition, methanol is a commodity and during a particularly mild winter its sale may prove to be profitable.

Figure 1 shows a block diagram of the overall process. Following the coal gasifier, sensible heat is removed from the hot gas in a heat recovery unit. After particles are scrubbed from the gas, sulfur is removed in a hydrogen sulfide selective acid gas process. This acid gas process should remove essentially all the sulfur compounds to prevent the methanol synthesis catalyst from being poisoned. Provision must be made downstream to remove final traces of residual sulfur compounds, if necessary. During the off-peak period, all or a portion of the desulfurized gas is directed to the methanol production unit where fuel grade methanol is produced and stored for later use. The gas stream rejected from the methanol unit is used to provide fuel to the base load combined cycle power train(s). During periods of peak demand all the desulfurized gas is diverted to the combined cycle power generation units. Additional combined cycle power trains, fueled by the previously stored methanol, would come on line to handle the peak load.

For this electric power and methanol combined process it is preferable that a gasifier be selected that produces a relatively small amount of carbon dioxide in the product gas. Otherwise, the excess carbon dioxide will need to be removed downstream at additional cost. Also for reasons of energy efficiencies it is desirable for the coal gasifier to operate at elevated pressure. Two examples of possible candidates which meet these criteria are the Shell gasifier and the British Gas/Lurgi Slagging gasifier.

THE METHANOL PRODUCTION UNIT

Although the hydrogen to carbon monoxide mole ratio of the gas leaving a suitable coal gasifier can be as low as 0.3:1, it should be as high as possible to maximize the amount of methanol produced. However, once the gasifier has been selected, the product gas hydrogen to carbon monoxide ratio is essentially fixed by the specific characteristics of the chosen gasifier. To make methanol from coal in a conventional process it would be necessary to par-

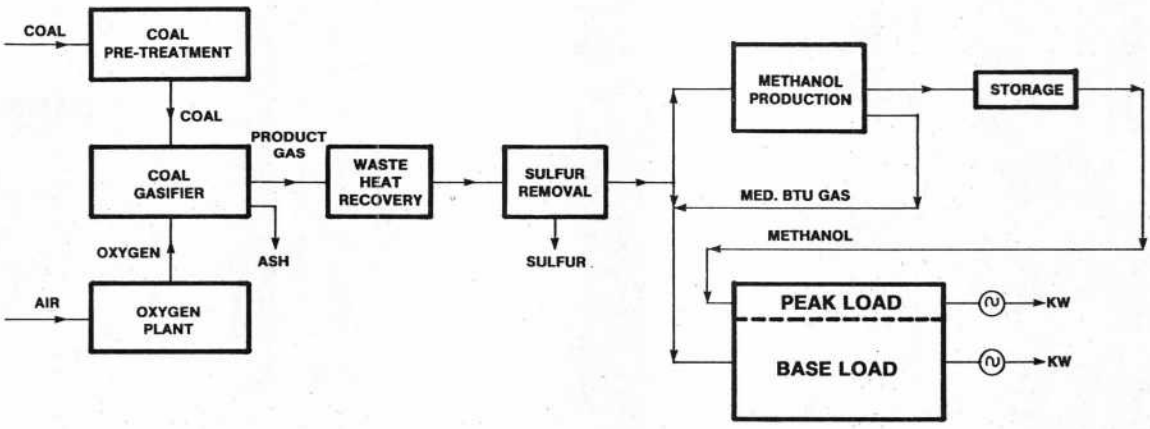

Figure 1. Process flow scheme for conversion of coal to power.

tially "shift" the gas (typically, over a sulfur tolerant catalyst) to achieve the preferred mole ratio:

$$\frac{H_2}{CO + 1.5\ CO_2} = 2.0$$

according to the following reaction:

$$CO + H_2O = H_2 + CO_2 \qquad \text{Shift Reaction}$$

In order for the Shift Reaction to proceed, the following need to occur: 1) excess steam has to be raised to drive the reaction forward and to moderate the temperature rise in the shift reactor, 2) a waste heat recovery unit is needed following the shift reactor, and 3) extensive condensate treatment is required prior to reusing the recovered condensate.

Furthermore, the fuel value of the converted carbon monoxide is lost in its conversion to carbon dioxide in the shift reactor. Also, this carbon dioxide will need to be removed at additional capital and operating expense. The carbon dioxide is removed in order to achieve the preferred stoichiometric ratio of reactants in the feed gas to the synthesis loop.

NEW CONCEPT

Figure 2 shows the flowsheet of a novel configuration for the methanol unit (patent pending). This unit would be built alongside a cogeneration or combined cycle process. The new configuration is intended to lower the initial investment and result in a plant which is simpler to operate compared to the conventional methanol process from coal. It differs from the conventional coal derived methanol process in that membrane separators (or pressure swing adsorbers) are used to eliminate the need for the CO shift reactor and associated equipment for steam raising, waste heat recovery, and condensate treating. The membranes (or PSA) concentrate the available hydrogen from both the feed gas and the noncondensible gas separated after the final methanol condenser, in order to achieve an optimum ratio of reactants in the methanol reactor.

An additional benefit of eliminating the CO shift reaction is that excess carbon dioxide is not produced as an unwanted by-product. This can lead to the elimination of the requirement for carbon dioxide removal if the coal gasifier does not produce too high a percentage of carbon dioxide in its product gas.

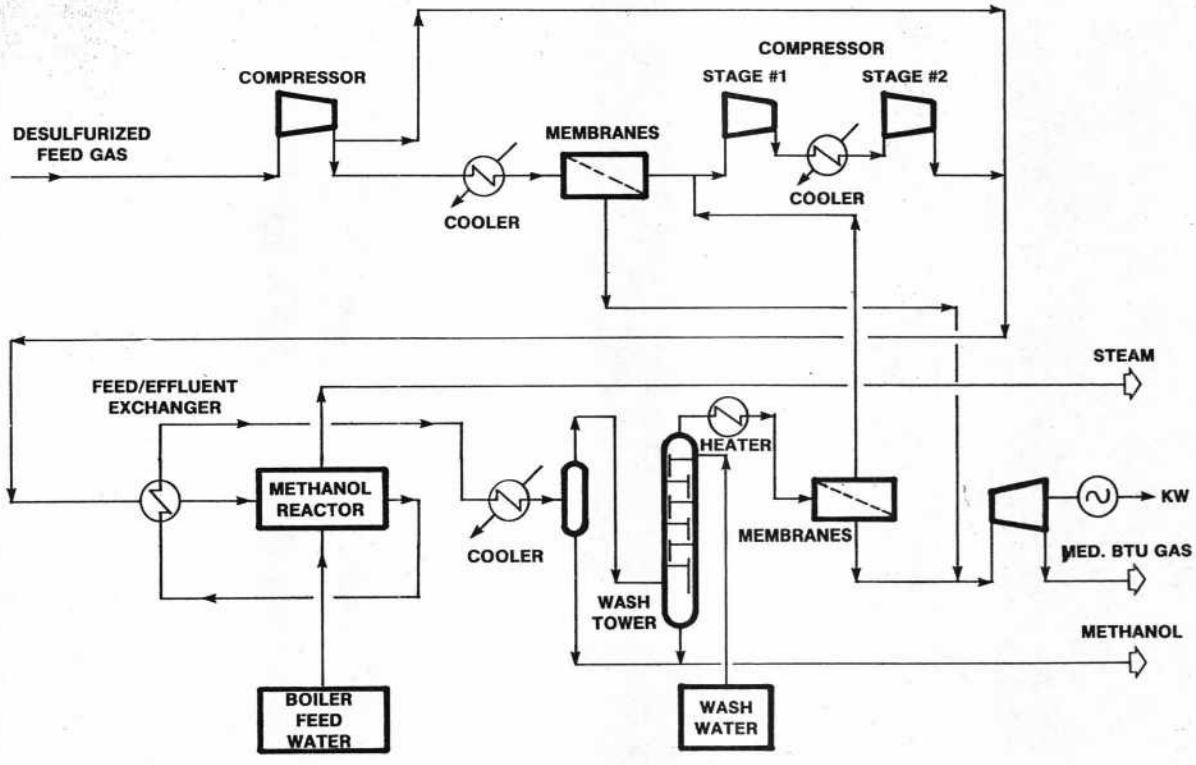

Figure 2. Methanol production.

PROCESS DESCRIPTION

Referring to Figure 2, sulfur free gas is cooled and compressed to about 760 psia (5240 kPa). Part of the compressed gas is cooled to ambient temperature prior to being fed to the first set of membrane separators. The hydrogen molecules will permeate faster through the membrane than the other constituents, producing a permeate stream relatively richer in hydrogen, and a non-permeate stream relatively leaner in hydrogen. By this mechanism, the membrane separators adjust the ratio of hydrogen to carbon monoxide and carbon dioxide.

The permeate stream is now joined by a second permeate stream rich in hydrogen from a downstream location and the combined stream is recompressed to about 750 psia (5168 kPa) in a two stage compressor. The discharge from the second compressor is combined with the flow of gas which by-passed the first set of membranes to achieve fine control of the required ratio of the reactants in the reactor.

The feed to the methanol reactor is preheated in the methanol feed/effluent heat exchanger. The methanol reactor used in this simulation was assumed to be an isothermal type. The outlet compositions in the reactor model are governed by the equilibria to the following chemical equations:

$$CO + H_2O = CO_2 + H_2$$
$$CO + 2H_2 = CH_3OH$$

Temperatures of approach were used to adjust the model to published operating data [3]. Since the reaction is exothermic the generated heat needs to be removed; this can be achieved by raising steam.

The hot gas leaving the reactor is cooled and partially condensed to form a condensate of mostly methanol and some water in a series of heat exchangers. Final traces of methanol vapor are removed from the uncondensed gas by a water wash. The washed gas is then warmed before being fed to the second set of membrane separators. The permeate stream leaving the second set of membranes is combined with the permeate stream from the first set of membranes upstream from the second compressor. Similarly, the two non-permeate streams are combined together, then let down in pressure to 250 psig (1825 kPa) across an expander coupled to a generator. The 250 psig (1825 kPa) gas is utilized as fuel in a downstream cogeneration or combined cycle unit.

RESULTS

Results from an earlier study and vendors' information were used to evaluate the overall penalty to efficiency caused by the integration of this methanol production process with a coal gasification and combined cycle power plant. The results from the earlier study establishes a benchmark for converting coal to power without the inclusion of a methanol unit. Vendor information was necessary to determine the practical efficiency that can be achieved when converting clean (sulfur free) fuel gas into power in a modern combined cycle system.

In 1980, H. K. Volkel, *et al.* [5] presented the results of an engineering study. In this study several processes to generate power from coal were compared, two of which are relevant to this work. One comprised a Shell-Koppers coal gasifier and waste heat recovery section integrated with a combined cycle power production system. The second process was a conventional, pulverized coal fired steam cycle with a stack gas non-regenerative scrubber to remove sulfur dioxide. Their results showed that the overall efficiency of converting the coal to electrical power (coal to busbar) at design load was 43.2% for the gasification route (including allowances for coal pulverization, oxygen production, sulfur removal, etc.). The overall efficiency for the conventional route is stated as 38.7%. Heat rates and efficiencies of power derived from coal are normally based on the gross heating value of coal.

A well designed, combined cycle, power production unit can convert a 300+ BTU/SCF gas at 45% efficiency [4]. Heat rates and efficiencies for gas turbines and combined cycles are normally based on the net heating value of the fuel. Using these efficiencies, it is possible to determine the impact on the overall plant heat rates (and efficiencies) while producing fuel grade methanol.

The overall heat rates and efficiencies can be determined from Table 1 and using the 45% efficiency figure. The 1000.00 MMBTU/hr (net basis) of desulfurized feed gas which can be either converted directly to power at 45% (7584 BTU/kWh net heating value basis), or it can be used to produce both power and methanol (which itself is convertible to power). In the first case, the power available is 131.857 MW, and in the second case the power available from the overall net product of 947.96 MMBTU/hr is 124.995 MW. The methanol coproduced in the process provides (168.51/947.96) × 100 = 17.8% of available power.

The combined cycle heat rates and efficiencies can not be compared directly with the results of the Volkel study (which is based on a bituminous coal of the Ruhr Area, West Germany), since the latter are based on a gross heating value. In the earlier study where no methanol was produced a heat rate (gross heating value basis) of 7900 BTU/kWh was obtained (equivalent to 43.2%). This would require 1041.67 MMBTU/hr (gross heat basis) of coal to produce the 131.877 MW of power available when the desulfurized gas is converted directly to power. During methanol production the coal rate stays the same, but the available power drops to 124.995 MW due to losses in the methanol production process. This means that the heat rate will increase to 8334 BTU/kWh (or that the efficiency will drop to 41.0% gross heating basis).

Summarizing the results (see Table 2), the net penalty on the overall production of power from coal while producing methanol for use during peak demand is a loss of 43.2-41.0 = 2.2% (gross basis). The trade-off is the convenience of being able to store up to 17.8% of the power in the form of methanol, or the added flexibility to sell the excess methanol produced as a commodity (assuming favorable economics). Even with the production and the ultimate total consumption of methanol into power, the overall con-

TABLE 1. OVERALL ENERGY BALANCE FOR METHANOL PRODUCTION UNIT
(Energy in Net Heating Value—MMBTU/Hr)

Input to Process	Products from Process	
Desulfurized Feed 1000.00	Non-Permeate Gas	789.47
	Methanol (liq) (19,594 #/hr)[1]	168.51
	Steam (from reaction)	22.55[2]
	Expander (2082 kw)[3]	15.79
	Sub-Total	996.32
	Internal Consumption	
	Comp #1 (1715 kW)[3]	13.01
	Comp #2 (4661 kW)[3]	35.35
	Sub-Total	48.36

Overall Net Product Available from Process 996.32-48.36 = 947.96

Notes:
[1]Methanol liq. net heating value = 8600 BTU/LB
[2]Exothermic heat removed by generating steam
[3]Conversion @ 45% Eff. i.e., 7584 BTU/kWh (net heating basis)

TABLE 2. SUMMARY OF OVERALL HEAT RATES AND EFFICIENCIES

	Coal	Desulfurized Gas		Power MW		Overall Heat Rate BTU/kWh	Overall Efficiency %
without methanol production	net basis	1000.00 MMBTU/hr		131.877		7584	45.0[2]
	gross basis 1041.67 MMBTU/hr			131.877		7900	43.2[1]
with methanol production	net basis	1000.00 MMBTU/hr	non-permeate 779.45 MMBTU/hr	102.775	82.2	7584	45.0[2]
			methanol 168.51 MMBTU/hr	22.191	17.8	7584	45.0[2]
			losses 52.04 MMBTU/hr	0	0	∞	0
			total	124.996	100.00	8000	42.7
	gross basis 1041.67 MMBTU/hr			124.996		8334	41.0
conventional steam cycle	gross basis 1041.67 MMBTU/hr			118.143		8817	38.7[1]

[1]Volkel [5].
[2]Combined cycle efficiency STAG™ [4].
[3]1 kWh = 3412.20BTU @ 100% efficiency.

version from coal to power is still more efficient compared to the conventional, pulverized coal steam cycle system with non-regenerative stack gas sulfur dioxide scrubbing.

MEMBRANE MODEL

Evaluation of new processes with flowsheet simulators requires the flexibility of adding new equipment models. These models may be too new to have been included in the flowsheet simulator, may be proprietary models, or may have certain characteristics required by the process. In this study the inline-FORTRAN processor was utilized to add a simple membrane separator model to the simulator. This processor made it possible to accept a FORTRAN subroutine directly into the input file containing the flowsheet model. DESIGN II[SM] automatically interfaces the routine to the flowsheet model, eliminating the need to perform compilation and linking steps.

The membrane model is based on equations presented in the literature [6] with the permeation rates back calculated from limited vendor data [2]. It assumes no change in feed temperature (which was the case in this simulation) and assumes that the relative permeation rates are held constant over the deviations from the set conditions provided by the vendor. Several runs were made and checked against the behavior given by the vendor's proprietary model. The results were sufficiently reliable to follow changes in the permeate compositions during the flowsheet recycle calculations.

CONCLUSIONS

Most of the reasons for promoting combined cycle over the conventional, pulverized coal fired steam cycle have been reported elsewhere in the literature [7]. They include: 1) projected installation costs are less than for a conventional power plant with the associated flue gas scrubber for the removal of sulfur dioxide; 2) combined cycle efficiencies are equal to if not greater than the conventional design; 3) high efficiencies and low costs are possible in smaller unit sizes than are possible in present day conventional power stations, resulting in reduced lead times in construction, and easier siting of the smaller facility; 4) gasification allows the use of high sulfur, low cost fuel in an environmentally acceptable manner and the sulfur can be recovered in a saleable form.

This methanol process is simple, lending itself to intermittent use during periods of base load power demand. Because the methanol reaction is carried out in the gas phase, the reactor design and catalyst could be provided by any one of the established licensors using proven technology.

The concept of concentrating hydrogen from a synthesis gas stream *vs.* the conventional shift reaction route can also be effectively applied to the co-production of SNG in a combined cycle (or cogeneration) facility. One possible flowsheet arrangement for SNG co-production is shown in Figure 3. From the simulation work carried out on this process, the conventional shift reactor (along with its necessary auxiliaries) and the conventional final methanator are not needed to produce an acceptable pipeline gas. The membranes serve to separate the available gas components instead of reacting them as would be the case in the shift and final methanator reactors.

One of the more costly units in the process are the sets of membrane separators. Membranes are relatively new and have not yet enjoyed the economies of scale in their manufacture. However, during just the past 24 months there has been a dramatic reduction in their costs. If this drop in price continues, then it will result in improved economics for this process.

Additional studies are required to more fully evaluate this process and its variations (such as the use of pressure swing adsorbers in place of the membrane separators), and to apply the concept to other processes.

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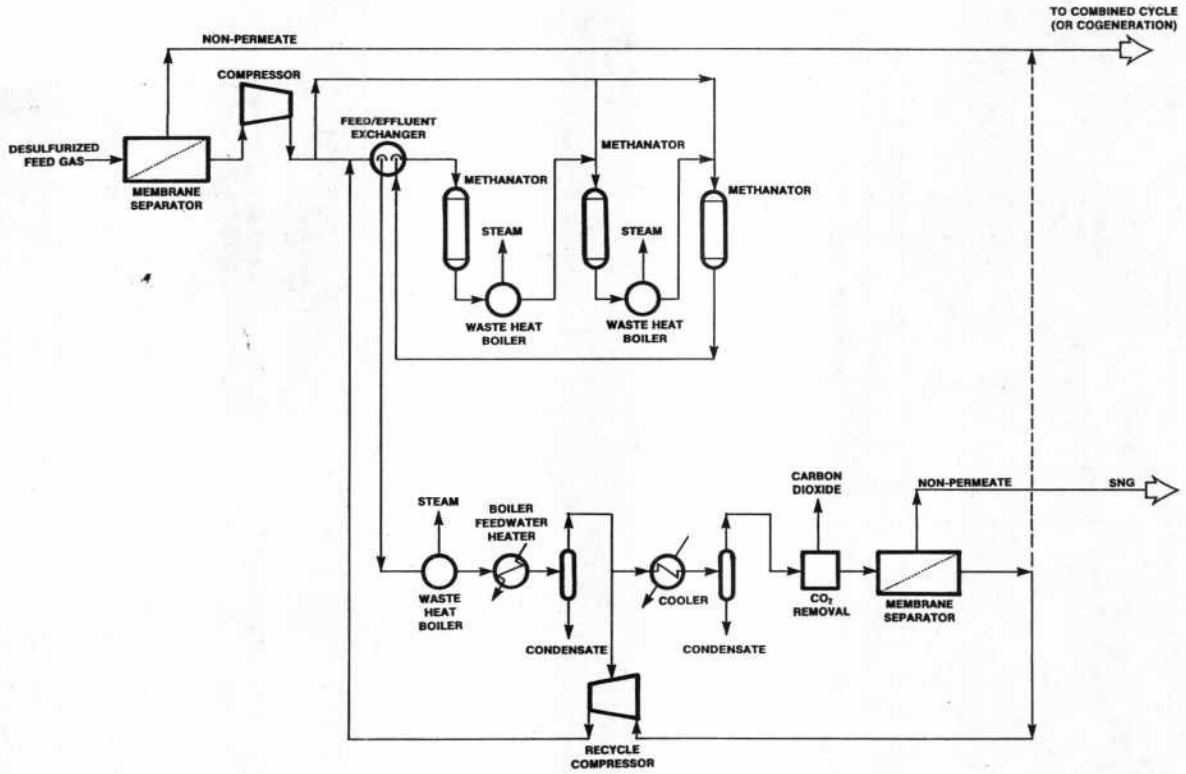

Figure 3. SNG production.

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