

MASS AND HEAT BALANCE FOR COAL GASIFICATION  
BY ATOMICS INTERNATIONAL'S MOLTEN SALT GASIFICATION PROCESS

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INTRODUCTION

Rockwell International's Atomics International (AI) Division is presently developing molten salt processes for the gasification of coal. In these processes, the coal is partially oxidized and completely gasified by reaction with air or with oxygen and steam in a bed of molten sodium carbonate. The gasification takes place at temperatures of 1700 to 1800°F and pressures of 10 to 30 atm. The sulfur and ash of the coal are retained in the melt. A nonpolluting low- or medium- Btu gas is produced which can be used as fuel gas for electric utility or industrial applications or as a synthesis gas for the production of pipeline quality gas, methanol, or liquid hydrocarbons. A sidestream of melt is withdrawn from the gasifier and processed in an aqueous regeneration system for removal of ash, recovery of elemental sulfur, and return of the regenerated sodium carbonate to the gasifier.

This report describes the mass and heat balance around the molten salt gasifier and the composition of the fuel gas produced as a function of air-to-coal or oxygen- and steam-to-coal feed ratios and system heat losses. Calculated values are compared with the experimental data obtained in laboratory and small scale pilot plant tests.

PROCESS DESCRIPTION

In the Molten Salt Coal Gasification Process, the coal is gasified at a temperature of 1700 to 1800°F and a pressure of 10 to 30 atm, depending upon the specific requirements of the process, by reaction with air or with oxygen and steam within a highly turbulent mixture of molten sodium carbonate containing sodium sulfide, ash, and unreacted carbon and coal. The sulfur and ash of the coal are retained in the melt, a sidestream of which is circulated continuously through a process system for regeneration of the carbonate, removal of the ash, and recovery of elemental sulfur. The fuel gas produced carries, as sensible heat, a major fraction of the heat released in the molten salt furnace and has an effective heating value of approximately 150 Btu/scf when the gasification is carried out with air or 300 Btu/scf when it is performed with oxygen and steam. Following cooling and scrubbing for removal of vaporized and entrained melt particulates, it can be used as a clean non-polluting fuel gas for electric utility or industrial applications, or as a synthesis gas for the production of pipeline quality gas, methanol or liquid hydrocarbons.

A steady-state concentration of ash and sulfur is maintained in the melt by the continuous withdrawal of melt from the gasifier and return of regenerated sodium carbonate back to the gasifier. The melt is quenched with water and processed in an aqueous regeneration system which removes the ash and sulfur compounds retained in the melt and returns the regenerated sodium carbonate back to the molten salt furnace. The ash is filtered out and disposed of in a conventional manner. The sulfur compounds are converted into hydrogen sulfide by carbonation of the aqueous solution, and the hydrogen sulfide thus released is, in turn, converted into elemental sulfur in a Claus plant. The sodium carbonate is regenerated as sodium bicarbonate which is filtered out of the solution and then calcined to yield sodium carbonate. The regenerated sodium carbonate and the makeup required to replace the small amount of salt lost in the process are returned to the molten salt furnace. The regeneration process is based, to a large extent, on technology presently in existence in the pulp and paper industry.

Figure 1 presents a schematic flow diagram of the process including gasification with either air or oxygen and steam to produce either low- or medium-Btu gas, respectively. The medium-Btu gas can be converted into pipeline quality gas (substitute natural gas, SNG) by water gas shift conversion and subsequent methanation.

Figure 2 shows an elevation of a typical small capacity molten salt gasifier. This is the gasifier for a 1 T of coal per hour Process Development Unit (PDU) presently being built at AI's field laboratory at Santa Susana, California, under contract to ERDA's Division of Coal Conversion and Utilization. All parts of the gasifier in contact with high temperature melt are fabricated of high purity alumina. Fusion cast alumina blocks such as Monofrax A\* are used as the primary lining in the melt area and high purity sintered alumina parts are used where special shapes or replaceable inserts are required, e.g., feed nozzles, heater and thermocouple shrouds, and melt discharge nozzle. Special features of the gasifier design include four down-sloping air-solids injection nozzles, a concept which has been verified by hydraulic testing, and a horizontal melt withdrawal chamber with auxiliary heaters. As shown in the drawing, the product gas is quenched in a spray cooler immediately after it leaves the gasifier. It is then further cooled and cleaned in a water scrubber. Pressure control on the gasifier system is maintained by control valves operating on the cooled gas.

A more detailed description of the PDU and of the status of the associated development program has been published in Reference 1.

#### BASIS AND ASSUMPTIONS

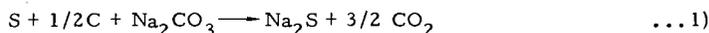
The following basis and assumptions are used to establish the mass and heat balance around the molten salt gasifier.

- 1) The mass and heat balance calculations are conducted on the basis of a unit mass of coal (for instance, 1 lb) being gasified. This makes the calculations almost completely independent of the capacity and design features of the gasifier. On this basis, the only parameter which is affected by the actual capacity and design features of the gasifier is the heat loss from the bed of molten salt to the environment through the walls of the gasifier vessel.
- 2) The temperature is uniform throughout the molten salt bed which behaves effectively like a three-phase fluidized bed with only negligible temperature gradients.
- 3) The operating pressure is the pressure of the product gas at the top surface of the molten salt bed.
- 4) With two exceptions, thermodynamic equilibrium conditions are assumed to prevail at the temperature and pressure of the gasifier. The equilibrium constants used were calculated from the free energy data published in the JANAF Tables.(2) They are plotted in Figure 3. All equilibrium calculations assume unit activity coefficients. It is to be noted that these equilibrium assumptions entail the assumption of complete utilization of the oxygen introduced into the gasifier.
- 5) The two exceptions involve the assumption of nonequilibrium conditions for CO<sub>2</sub> in the presence of carbon and CO, and for CH<sub>4</sub> in the presence of CO (or carbon) and H<sub>2</sub>. With respect to the CO<sub>2</sub>, CO, and carbon, this means that unreacted carbon is assumed to be present in the melt even though the CO<sub>2</sub> content of the gas exceeds that which would be predicted on the basis of thermodynamic equilibrium.

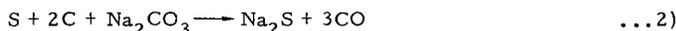
\*Trademark of the Carborundum Company

6) Atmospheric pressure and low pressure gasification tests have generally shown the presence of methane in the product gas at concentrations (1 to 2 mole %) considerably above those one would expect to find on the basis of thermodynamic equilibrium. This may be attributable to incomplete cracking of the volatile matter of the coal in the relatively small test units. For purposes of calculation, the mass balance relationships have been written to allow insertion of an arbitrarily selected (on the basis of test data) value,  $\alpha$ , for the methane concentration of the product gas. It is expected that actual adjusted equilibrium data will be used at a later date when additional test information has become available.

7) The sulfur of the coal behaves as elemental sulfur (the Dulong formula provides for a heating value contribution of 4000 Btu/lb, equivalent to the enthalpy of oxidation of sulfur to  $\text{SO}_2$ ). A major fraction of this sulfur is assumed to react with the sodium carbonate of the melt to form sodium sulfide according to the following stoichiometry:

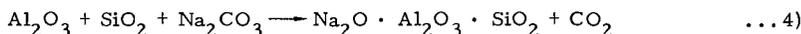
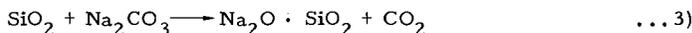


It is to be noted that the stoichiometry would effectively be the same if the reaction had been assumed to be



In both cases, a mole of sulfur reacts to release 1 atom of carbon and 3 atoms of oxygen from the sodium carbonate into the product gas.

8) Both the silica and the alumina of the ash of the coal react completely with the sodium carbonate to form sodium silicate and sodium aluminum silicate, releasing 1 mole of  $\text{CO}_2$  per mole of  $\text{SiO}_2$  (assuming an excess of silica) from the sodium carbonate into the product gas:



9) To simplify the calculations, the initial mass balance takes into account only the major constituents of the product gas ( $\text{CO}$ ,  $\text{H}_2$ ,  $\text{CH}_4$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$ ). The concentrations of the minor constituents ( $\text{H}_2\text{S}$ ,  $\text{COS}$ ,  $\text{Na}$ ,  $\text{NaOH}$ ) are then calculated on the basis of the equilibrium data and an iteration is made to provide for second order corrections to the concentrations of the major constituents. The presence of ammonia is neglected since its concentration has always been found to be <5 ppm.

10) The reference air composition used in these calculations includes moisture (60% of saturation at 80°F) and groups the argon in with the nitrogen.

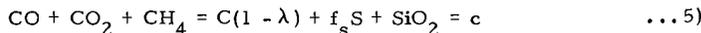
11) The definitions of the symbols used are given in the table of nomenclature at the end of this report.

## MASS BALANCE

### 1. Fuel Gas Composition

The following five equations are used in the mass balance around the gasifier:

Carbon Balance (lb moles per lb coal)



Hydrogen Balance (lb moles per lb coal)

$$H_2 + H_2O + CH_4 = H + M + 0.02053A + St = h \quad \dots 6)$$

Oxygen Balance (lb moles per lb coal)

$$CO + 2CO_2 + H_2O = 2O + M + 3f_s S + 2SiO_2 + 0.4312A + 2f_{ox} O_x + St = b \quad \dots 7)$$

Nitrogen Balance (lb moles per lb coal)

$$N_2 = N + 0.7741A + (1 - f_{ox})O_x = h \quad \dots 8)$$

Water Gas Shift Equilibrium

$$\frac{[H_2][CO_2]}{[H_2O][CO]} = K_1 \quad \dots 9)$$

If one defines:

$$\Sigma = \frac{c + h + n}{1 + 2\alpha} \quad \dots 10)$$

$$q = (1 - \alpha)\Sigma - b - n \quad \dots 11)$$

$$s = c - \alpha\Sigma \quad \dots 12)$$

$$w = \frac{K_1 b + q}{2(1 - K_1)} \quad \dots 13)$$

$$x = w \left[ \sqrt{1 + \frac{K_1}{1 - K_1} \frac{s(b - s)}{w^2}} - 1 \right], \quad \dots 14)$$

the composition (major constituents) of the product gas is derived from:

$$[CO] = (s - x)/\Sigma \quad \dots 15)$$

$$[H_2] = (q + x)/\Sigma \quad \dots 16)$$

$$[CH_4] = (c - s)/\Sigma = \alpha \quad \dots 17)$$

$$[CO_2] = x/\Sigma \quad \dots 18)$$

$$[H_2O] = (b - s - x)/\Sigma \quad \dots 19)$$

$$[N_2] = n/\Sigma \quad \dots 20)$$

It is to be noted that  $\Sigma$  represents the number of lb moles of product gas per lb of coal and that  $\alpha$  is the arbitrarily assumed concentration of methane in this gas, selected on the basis of experimental data.

The minimum amount of air or oxygen which is theoretically required to gasify the coal can be derived from the above relationships for the case in which  $[\text{CO}_2] = [\text{H}_2\text{O}] = 0$ ; hence

$$b - s = 0 \quad \dots 21)$$

## 2. Melt Composition

The sodium carbonate feed to the gasifier (recycle from regeneration system plus makeup) required to maintain a specified steady-state ash concentration in the melt is given by

$$R = \frac{1 - a_m}{a_m} \frac{a_c}{105.989} \quad \dots 22)$$

In this equation, R is the sodium carbonate feed in lb moles per lb of coal,  $a_c$  is the ash content of the coal and  $a_m$  is the "nominal" steady-state ash content of the melt based on the unreacted ash of the coal and the unreacted sodium carbonate feed.

The composition (major constituents) of the melt is obtained from the following relationships:

$$\left. \begin{aligned} \text{Na}_2\text{CO}_3 &= R - f_s S - \text{SiO}_2 && \dots 23) \\ \text{Na}_2\text{S} &= f_s S && \dots 24) \\ \text{Na}_2\text{O} \cdot \text{SiO}_2 &= \text{SiO}_2 - \text{Al}_2\text{O}_3 && \dots 25) \\ \text{Na}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot \text{SiO}_2 &= 224.025 \text{ Al}_2\text{O}_3 && \dots 26) \\ \text{Unreacted carbon} &= 12.011 \text{ C} && \dots 27) \\ \text{Unreacted ash} &= a_c - 60.085 \text{ SiO}_2 - 101.961 \text{ Al}_2\text{O}_3 && \dots 28) \end{aligned} \right\} \begin{array}{l} \text{lb moles/} \\ \text{lb coal} \\ \\ \\ \text{lb/lb coal} \end{array}$$

The first three compounds are assumed to constitute the liquid phase of the melt, while the sodium-aluminum-silicate, the unreacted carbon, and the unreacted ash constitute its insoluble solid phase. The actual situation is considerably more complex with some of the sodium sulfide believed to be retained in the solid phase in the form of compounds of the type  $\text{Na}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot \text{SiO}_2 \cdot (\text{Na}_2\text{S})_n$ .

The fraction of unreacted carbon,  $\lambda$ , can be calculated from its concentration in the melt,  $c_m$ , by the following relationship:

$$\lambda = \frac{c_m}{1 - c_m} \frac{a_c + 105.989 R - 27.945 f_s S - 44.010 \text{ SiO}_2}{12.011 \text{ C}} \quad \dots 29)$$

$$= \frac{c_m}{1 - c_m} \frac{\frac{a_c}{a_m} - 27.945 f_s S - 44.010 \text{ SiO}_2}{12.011 \text{ C}} \quad \dots 30)$$

### 3. Minor Constituent Adjustments

The minor constituent concentrations are calculated on the basis of the thermodynamic equilibria using the previously obtained major constituent concentrations and going through a second iteration (if necessary) after adjusting the major constituent concentrations for the calculated amounts of minor components.

The following relationships prevail:

$$\left. \begin{aligned} [\text{H}_2\text{S}] &= K_4 \pi [\text{CO}_2] [\text{H}_2\text{O}] \frac{[\text{Na}_2\text{S}]}{[\text{Na}_2\text{CO}_3]} & \dots 31) \\ [\text{COS}] &= K_5 \pi [\text{CO}_2]^2 \frac{[\text{Na}_2\text{S}]}{[\text{Na}_2\text{CO}_3]} & \dots 32) \\ [\text{Na}] &= \frac{1}{\pi} \sqrt{\frac{K_6}{\pi} \frac{[\text{CO}]}{[\text{CO}_2]^2} [\text{Na}_2\text{CO}_3]} & \dots 33) \\ [\text{NaOH(g)}] &= \frac{1}{\pi} \sqrt{K_7 \frac{[\text{H}_2\text{O}]}{[\text{CO}_2]} [\text{Na}_2\text{CO}_3]} & \dots 34) \\ [\text{NaOH(l)}] &= \sqrt{K_8 \frac{[\text{H}_2\text{O}]}{[\text{CO}_2]} [\text{Na}_2\text{CO}_3]} & \dots 35) \end{aligned} \right\} \begin{array}{l} \text{Gas Phase} \\ \text{Liquid Phase} \end{array}$$

It is to be pointed out that the sodium and sodium hydroxide vapors are expected to react and condense into sodium carbonate particulates when the gas is cooled downstream of the gasifier. The concentration of these particulates will decrease with increasing pressure. The concentration of  $\text{H}_2\text{S}$  and  $\text{COS}$  on the other hand will increase with increasing pressure.

### HEAT BALANCE

The heat balance around the molten salt in the gasifier takes into account the following inputs, outputs, and losses, measured, when appropriate, above a reference temperature of  $60^\circ\text{F}$  (water in liquid form).

#### 1) Heat Input

- a) Higher heating value and enthalpy of coal feed.
- b) Enthalpy of air (or oxygen) feed, including latent heat of moisture in air.
- c) Enthalpy of steam feed.

#### 2) Heat Output

- a) Higher heating value and enthalpy of product gas.
- b) Enthalpy of discharge melt.

3) Heat Losses

- a) Unrealized heats of combustion.
- b) Endothermic heats of reaction.
- c) Heat losses from the melt to the environment through the walls of the gasifier vessel.

The heat balance around the melt in the gasifier can now be written

$$Q_{In} = HHV_{Coal} + H_{Coal} + H_{Air} + H_{Ox} + H_{St} \quad \dots 36)$$

$$Q_{Out} = HHV_{Gas} + H_{Gas} + H_{Melt} \quad \dots 37)$$

$$Q_{Loss} = Q_{Unreacted} + Q_{Reaction} + Q_{Gasifier} \quad \dots 38)$$

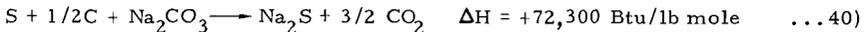
$$Q_{In} = Q_{Out} + Q_{Loss} \quad \dots 39)$$

The heat input and heat output calculations are quite straightforward once the compositions of the feed and discharge streams have been established. The enthalpy data are taken from the JANAF Tables.<sup>(2)</sup>

Calculation of heat losses deserves amplification. The unrealized heats of combustion involve the unreacted carbon of the coal and its uncombusted sulfur. The sulfur does not only remain uncombusted, but is reduced to sulfide, utilizing some of the carbon for the reduction and absorbing heat through this endothermic reaction.

The unreacted carbon heat loss amounts to 169,300  $\lambda$  C Btu/lb of coal, equivalent to 141 Btu/lb of coal per percent unreacted carbon (the percent in this case is based on the total coal).

The heat loss associated with the reduction of the sulfur to sulfide can be calculated by taking the difference between the enthalpies of reaction of the reduction reaction and of the normal combustion reaction:



The net result is a heat loss of 284,600  $f_S$  Btu/lb of coal, equivalent to 88.8 Btu/lb of coal per percent sulfur reduced to sulfide (the percent here is again based on the total coal).

Additional endothermic reaction heat losses are associated with the enthalpies of reaction of the silica and alumina of the coal ash with the sodium carbonate of the melt. These amount to (36,200 SiO<sub>2</sub> + 62,900 Al<sub>2</sub>O<sub>3</sub>) Btu/lb of coal, equivalent to 6.03 (% SiO<sub>2</sub>) + 6.17 (% Al<sub>2</sub>O<sub>3</sub>) Btu/lb of coal, with the percent again based on the total coal.

Other heat losses (and gains) are associated with the reactions of formation of the minor constituents of the gas and melt. These have generally been small enough to be negligible in the overall calculations.

The heat loss from the melt to the environment through the walls of the gasifier vessel is the only component of the heat balance which is a function not only of the process conditions but mainly of the capacity and design features of the gasifier. For gasifiers with similar design features operating under similar conditions, this loss, when normalized to 1 lb of coal, is an inverse function of the coal processing capacity of the gasifier. For AI's test gasifier operating at atmospheric pressure with a coal throughput of 200 lb/h, this heat loss amounts to 1700 Btu/lb of coal. For ERDA's PDU at Santa Susana, this loss is reduced to 200 Btu/lb of coal when operating at a throughput of 1 T/h. It is expected to be in the range of 50 to 100 Btu/lb of coal in gasifiers with throughputs in excess of 10 T/h.

## RESULTS

### 1. Typical Mass and Heat Balance Calculations

Figures 4 and 5 show plots of the calculated gasifier melt heat balance for the gasification of Kentucky No. 9 (4.3% sulfur, 15% ash, 11,408 Btu/lb) coal with air and steam at 1800°F, and the gasification of Kentucky No. 9 coal and Elkhorn No. 3 (1% sulfur, 8% ash, 13,354 Btu/lb) coal with oxygen and steam at 1800°F. In both figures the heat input and output are plotted as a function of air (or oxygen)-to-coal feed ratios at constant steam-to-air (or oxygen) feed ratios. The heat input includes the heating value and enthalpy of the feed streams. The heat output includes the heating value and enthalpy of the output streams (calculated from the composition data obtained from the mass balance calculations) plus the heat losses. The intersections of the respective input and output lines provide the operating conditions for operation at 1800°F.

It is interesting to note that in the gasification of Kentucky No. 9 coal with air there is no advantage in adding steam to the process. The presence of the steam only decreases the heating value of the product gas.

In the gasification of Kentucky No. 9 coal with oxygen, steam is not required, but its addition allows operation of the gasifier under conditions providing an appreciable excess margin of oxygen and steam over the minimum required for gasification, without appreciably decreasing the heating value of the product gas. The oxygen gasification of Elkhorn No. 3 coal cannot be accomplished at 1800°F without the addition of steam.

Table 1 shows the calculated coal gasification data for the gasification of Kentucky No. 9 and Elkhorn No. 3 coals with oxygen. The oxygen- and steam-to-coal feed ratios were selected on the basis of the heat balance of Figure 5 to produce a fuel gas with a higher heating value of about 320 Btu/scf (dry).

### 2. Experimental Data

The experimental data on the composition of the product gas as a function of air (or oxygen)-to-coal and steam-to-coal feed ratio have generally confirmed the values calculated by the above described mass and heat balance calculation procedures. A detailed analysis of the data obtained as a function of test conditions is beyond the scope of this report. Table 2 presents a comparison of calculated and measured product gas composition data for the gasification of Kentucky No. 9 coal with oxygen and steam at atmospheric pressure and temperatures of 1700 to 1800°F in a laboratory gasifier. The main difference appears to be in the CO and CO<sub>2</sub> concentrations,

TABLE 1  
CALCULATED COAL GASIFICATION DATA  
GASIFICATION OF KENTUCKY No. 9 AND ELKHORN No. 3 COALS  
WITH OXYGEN AND STEAM

Coal	Kentucky No. 9	Elkhorn No. 3
Oxygen, lb/lb coal	0.66	0.70
Steam, lb/lb coal	0.11	0.35
Product gas, lb/lb coal	1.67	2.00
scf/lb coal	30.5	39.1
Product Gas Composition		
CO, volume %	58.3	52.2
H <sub>2</sub> , volume %	28.5	33.4
CH <sub>4</sub> , volume %	2.5	2.5
CO <sub>2</sub> , volume %	5.6	5.6
H <sub>2</sub> O, volume %	4.4	5.7
N <sub>2</sub> , volume %	0.7	0.6
H <sub>2</sub> S, ppm	248	100
Product Gas HHV, Btu/scf wet	305.3	301.9
dry	319.1	320.0

TABLE 2  
PRODUCT GAS COMPOSITION  
GASIFICATION OF KENTUCKY NO. 9 COAL WITH OXYGEN AND STEAM

Coal, lb/h	6.59		7.20		6.86		7.70		7.70	
Oxygen, lb/h	4.30		4.30		4.26		4.28		4.26	
Steam, lb/h	1.83		1.83		0.93		1.39		0.93	
Temperature, °F	1794		1801		1719		1737		1720	
Gas Composition vol % dry basis	Calc.	Actual								
	CO	52.7	49.8	54.9	49.6	60.4	53.3	59.3	53.9	62.8
H <sub>2</sub>	33.1	34.3	34.0	34.5	31.2	33.8	33.7	33.3	32.5	33.1
CH <sub>4</sub>	2.8	2.1	2.7	2.5	2.6	2.4	2.6	2.4	2.5	2.0
C <sub>2</sub> H <sub>6</sub>	—	0.2	—	0.3	—	0.2	—	0.5	—	0.4
CO <sub>2</sub>	10.7	12.4	7.7	12.1	5.1	9.5	3.7	9.3	1.5	8.2
N <sub>2</sub>	0.7	1.1	0.7	1.0	0.7	0.7	0.7	0.6	0.7	0.8
Higher Heating Value, Btu/scf	304	296	314	302	322	309	326	314	333	313

with the product gas containing 6 to 12% less CO than predicted and correspondingly more CO<sub>2</sub>. The difference may possibly be attributable to a slightly higher oxygen feed rate than shown by the flow rate measured during the tests.

Figure 6 is presented to show typical experimentally obtained higher heating values (HHV) of the fuel gas produced during a 15-day atmospheric pressure air gasification test of Kentucky No. 9 coal at temperatures ranging from 1661 to 1945° F plotted as a function of air-to-coal feed ratio. This test was conducted at AI's Molten Salt Test Facility pilot plant at Santa Susana, California. The solid and dashed curves show the expected values of the HHV based on the predicted compositions of the product fuel gas. The sodium carbonate addition and melt withdrawal rate were varied over a wide range during this test. The unreacted carbon loss associated with the melt withdrawal varied accordingly. The effect of this variation is shown by plotting the solid and dashed curves to cover the range of anticipated unreacted carbon loss. It can be seen that the data points in general follow the curves quite well, with most of them falling well within the expected precision of the experimental measurements.

### CONCLUSION

The calculational procedures described in this report provide the necessary means for developing a first approximation model of the operation of the molten salt gasifier. While the experimental work has confirmed the applicability of these procedures to the analysis of the performance of laboratory-scale and small pilot plant-scale gasification tests, additional work needs to be done to develop a better definition of methane production and of the effect of operation at elevated pressures (10 to 30 atm). The predicted effects of pressure on methane production, hydrogen sulfide release from the melt, and emission of particulates by vaporization of melt components remain to be confirmed experimentally. It is planned that this information be developed in the next year through gasification tests to be conducted in the laboratory pressurized gasifier presently under construction at Atomic International.

### TABLE OF NOMENCLATURE

A	Gasification air, lb moles/lb coal
a <sub>c</sub>	Ash content of coal, lb/lb coal
a <sub>m</sub>	Nominal ash content of discharge melt, lb/lb melt
b	Parameter defined in text
c <sub>m</sub>	Unreacted carbon content of discharge melt, lb/lb melt
f <sub>ox</sub>	Gasification oxygen purity, volume fraction O <sub>2</sub> in oxygen used
f <sub>s</sub>	Fraction of coal sulfur reacted to form Na <sub>2</sub> S
H	Enthalpy of coal, air, oxygen, steam, product gas or melt above a given reference temperature (60°F), including latent heat of water vapor, Btu/lb coal (except in Equation 6 where it denotes lb moles hydrogen per lb coal)
HHV	Higher heating value of coal or fuel gas, Btu/lb coal
h	Parameter defined in text
K	Thermodynamic equilibrium constants
M	Moisture content of coal, lb moles/lb coal

- n Parameter defined in text
- Ox Gasification oxygen, lb moles/lb coal
- Q Heat input into melt, heat output from melt, or heat losses from unreacted combustibles, endothermic reactions, and through the walls of the gasifier vessel.
- q Parameter defined in text
- R Sodium carbonate recycle to gasifier, lb moles/lb coal
- s Parameter defined in text
- St Gasification steam, lb moles/lb coal
- w Parameter defined in text
- x Parameter defined in text
- $\alpha$  Mole fraction methane in product gas
- $\lambda$  Fraction unreacted carbon
- $\pi$  Gasifier pressure, atm
- $\Sigma$  Total fuel gas production, lb moles/lb coal

Chemical symbols and formulae. Wherever chemical symbols and formulae are used outside of chemical reactions, they represent lb moles of the element or compound per lb of coal. (C, H, N, O, S,  $\text{Al}_2\text{O}_3$ ,  $\text{SiO}_2$ ) are used to denote the amounts of the respective elements or compounds present in the coal, [ $\text{CH}_4$ , CO,  $\text{CO}_2$ ,  $\text{H}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{N}_2$ ,  $\text{H}_2\text{S}$ , COS, Na,  $\text{NaOH}(\text{g})$ ] denote the amounts of the respective elements or compounds in the product gas, and [ $\text{Na}_2\text{CO}_3$ ,  $\text{Na}_2\text{S}$ ,  $\text{NaOH}(\text{l})$ ,  $\text{Na}_2\text{O} \cdot \text{SiO}_2$ ,  $\text{Na}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot \text{SiO}_2$ ] represent the amounts of the respective elements or compounds in the product gas, and [ $\text{Na}_2\text{CO}_3$ ,  $\text{Na}_2\text{S}$ ,  $\text{NaOH}(\text{l})$ ,  $\text{Na}_2\text{O} \cdot \text{SiO}_2$ ,  $\text{Na}_2\text{O} \cdot \text{Al}_2\text{O}_3 \cdot \text{SiO}_2$ ] represent the amounts of the respective elements or compounds in the melt discharge from the gasifier.

#### REFERENCES

- (1) W. V. Botts, A. L. Kohl, and C. A. Trilling, "Low-Btu Gasification of Coal by Atomics International's Molten Salt Process," Proceedings of the 11th Intersociety Energy Conversion Engineering Conference, Volume I, pp 280-285 (September 12-17, 1976)
- (2) D. R. Stull and H. Prophet, "JANAF Thermochemical Tables, Second Edition," NSRDS-NBS37, National Bureau of Standards, U. S. Department of Commerce (June 1971)

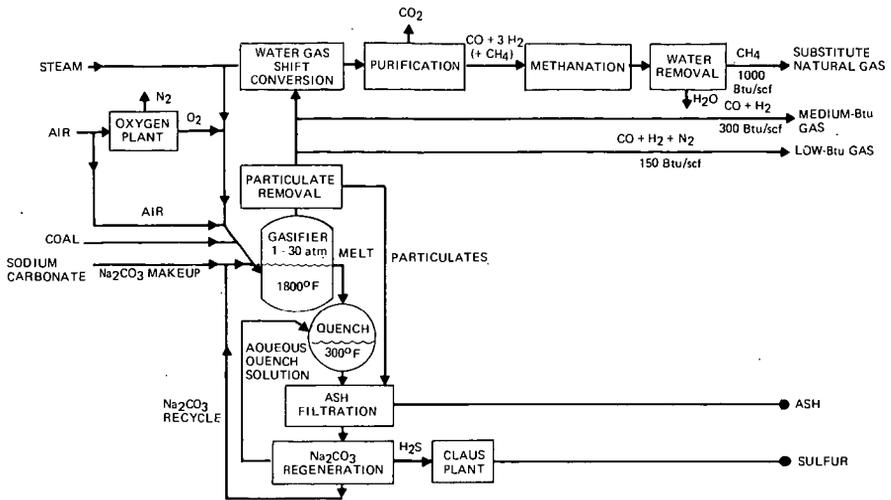


Figure 1. Molten Salt Gasification of Coal

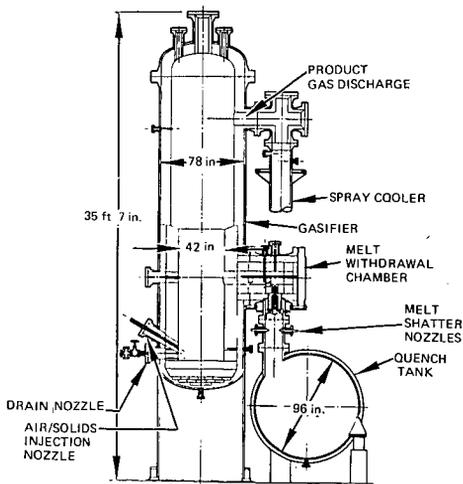


Figure 2. PDU Gasifier Assembly

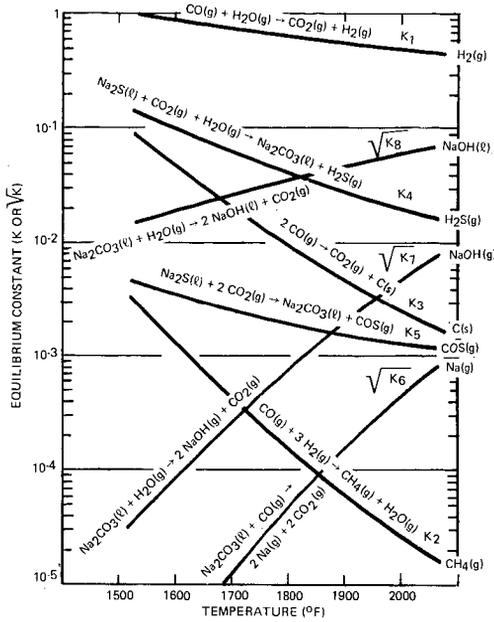


Figure 3. Molten Salt Coal Gasification Equilibrium Constants

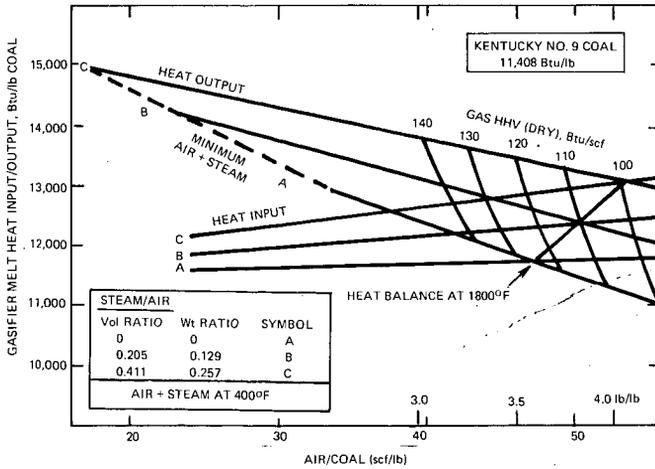


Figure 4. Air-Steam Gasification Heat Balance at 1800°F

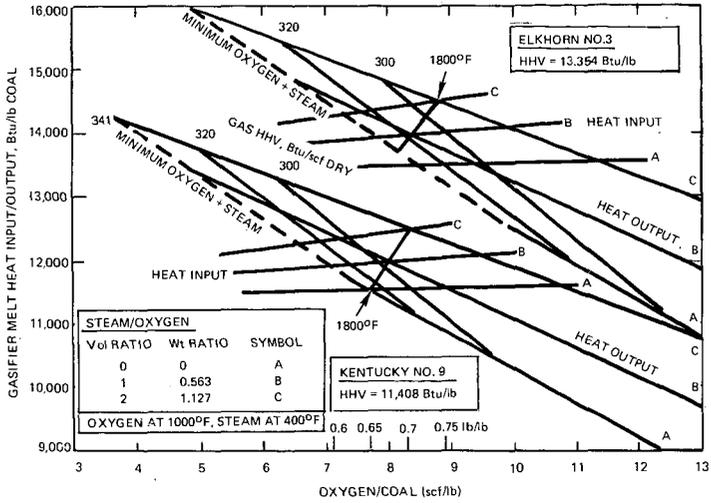


Figure 5. Oxygen-Steam Gasification Heat Balance at 1800°F

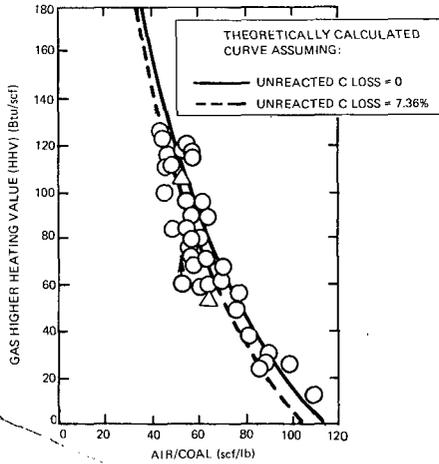


Figure 6. Higher Heating Values of Product Gas as a Function of Air-to-Coal Feed Ratio  
Air Gasification of Kentucky No. 9 Coal