**Quarterly Summary Report
April - June 1977**

**Process for Cleaning and Removal
of Sulfur Compounds from
Low Btu Gases**

by
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July 21, 1977

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BATTELLE
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I. OBJECTIVE AND SCOPE OF WORK PHASE IV

In this phase of work the Process Development Unit (PDU) is to be remodeled by incorporation of appropriate subsystems to permit operation in continuous process mode. The PDU will be operated for a period of time sufficient to demonstrate process viability.

II. SUMMARY

1) Pending return of "Alonized" pipe and equipment, the following tasks were completed:

- a) Lock hopper and conveyor were placed in operational readiness.
- b) Insulation on the gasifier and on air-steam inlet and gas outlet lines has been repaired.
- c) The tar trap has been installed.
- d) The air preheater and steam-CO₂ preheater have been fabricated and the former has been installed and trace heaters mounted, but not electrically connected.
- e) A subcontract for installation of part of the electrical equipment has been negotiated. The equipment is on hand and work is to be completed by mid-August.
- f) Design of the analytical sampling system has been completed and difficulties with the determination of low H₂S concentrations in steam-CO₂ mixtures resolved.

2) A portion of the equipment to be "Alonized" was received from Alon Processing Inc. on June 27, 1977. The remainder of the order is expected about mid-July--some six weeks beyond the most optimistic delivery date. The project

schedule is delayed accordingly. To the extent possible this equipment is being installed on the support structure. Installation will be completed as soon as all of the parts are received.

3) Computer modeling is complete except for writing instructions which anyone skilled in computer modeling could employ.

III. TECHNICAL PROGRESS

A. Maintenance of Operational Readiness

The long period of idleness and exposure to weather has caused less damage to components of the Battelle gasifier than was expected. It was only necessary to connect the air supply to the pneumatic slide valves on the lock hopper, apply a little oil, and response to both manual and automatic controls was immediate. The conveyor responded by shearing a pin and it was found that the drive motor was wired incorrectly (a result of the move to the Chemical Engineering Lab). This was easy to correct. A small air preheater which heats the air entering the gasifier to 350-450°F (to prevent condensation of steam which combines with the entering air) was regasketed. A new thermocouple was installed, and the controller wiring checked.

Finally, the insulation on air and steam lines leading to the gasifier and on exit lines was repaired. The Columbia Ground Squirrel which infests this area has a taste for pipe insulation--evidently to line nesting areas in their burrows. Their depredations over the past year or more has severely damaged the insulation. This has now been replaced and sheathed in an outer covering of aluminum sheet metal which should reduce the attractiveness so far as the rodents are concerned.

B. Construction and Assembly

A tar trap has been installed in the 6-in. line through which product gases emerge from the gasifier. This unit is evident in the photo (Figure 1) which also shows some of the insulation referred to above. The tar trap has sufficient capacity to hold tars and oils from gasification of about a ton of coal and will have to be drained once per day. A gate valve and 2-in. line leading to a steel drum will enable removal of tars and oils with no personnel exposure.

FIGURE 1. Photo Showing Tar Trap Installation

It is not anticipated that this unit will be sufficiently effective to remove all tars and oils, so the molten salt scrubber will be tested adequately for effectiveness in their removal. The unit should be sufficient to ensure that lines leading to the scrubber remain clear for reasonable periods and that the gas preheater is not severely fouled.

The tars and oils which reach the throat of the venturi will be subjected to intimate contact with the dispersed salt and should track with the salt phase as it coalesces and de-entrains. At 700°C pyrolysis and cracking reactions should proceed with production of low molecular weight hydrocarbons and char. If the char floats it will concentrate at the surface of the venturi feed tank and overflow with salt bled intermittently from this tank.

Addition of makeup salt to replace that bled from the venturi feed tank is to be done by adding solid salt in small amounts to the salt held in the large salt makeup pot. This pot and its large (45 kW) furnace is to be used in melting the inventory of salt (5400 lb). With some 200 lb of salt resident at all times in this pot, addition of 10 lb increments on occasion will have little effect on the temperature of the salt leaving the bottom of the pot. Addition of salt does pose a problem, however, because the salt makeup pot cannot be opened for salt addition without causing loss of steam-CO₂ flow (pressure) in the regeneration column. It was therefore necessary to provide a small lock hopper (Figure 2) which sits atop the salt makeup pot through which salt can be added. The lock hopper consists of a small spool piece capped by a 6 in. blind flange which can easily be removed. This assembly sits above a 6 in. slide valve which, when opened, allows salt to fall into the pot.

The air preheater described in last quarter's report has been assembled and mounted on the support structure. The air supply line, including a motor driven valve for flow control, has been connected. Trace heaters have been installed but the controller has not been connected (although it is ready for installation). Figure 3 shows the air preheater with a layer of plastic protecting the trace heaters until insulation and weatherproof cover is installed. The steam-CO₂ preheater is partially visible at the left.

FIGURE 2 Photo Showing Lock Hopper Salt Makeup Additions

FIGURE 3. Air Preheater Complete with Trace Heaters Installed.
A Portion of the Steam-CO₂ Heater is at Lower Left.

A part of the electrical work will be performed under subcontract and this work should commence in a few days. This work includes installation of transformers, relays, and relay mounting boxes, circuit breakers, controllers, and wire ways. Our electricians and instrument men will install thermocouples and trace heaters and will test and certify operability of all installations.

On June 27, 1977, we received a partial shipment of our "Alonized" pipe and equipment. Only major equipment pieces were shipped. All 1-in. and 2-in. pipe, the venturi, and key parts of the 4-in. line were missing. Alon Processing reported these items were shipped on June 29, 1977, but as yet they have not arrived (July 8, 1977).

We have assembled and mounted all major equipment pieces on the support structure. These pieces include the extraction column and packed bed de-entrainer, the regeneration column, coarse de-entrainer, venturi feed tank, and 24-in. dia x 24-in. deep salt makeup pot. Piping connections cannot be made until all pieces are available.

A residue of $Al-Al_2O_3$ (loosely adherent) was found to be present on all surfaces of the pipe and equipment. This was removed to the extent possible with brushes, high pressure air, and water.

Before the equipment is all buttoned up, it is convenient to calibrate tank volumes using water. This has been completed. It is also planned to operate the extraction and regeneration columns (using air and water) to get pressure drop readings across the trays and to get column holdup volumes. Any fouling of blind sections of the regenerator by debris from the "Alonizing" step will be detected.

Sampling and analysis are critically important to the success of this program. Two isokinetic samplers and two Anderson-2000 impingers are available for taking inlet and outlet particle samples. These will yield total particle burden and particle size distribution. These devices also allow measurement of the average moisture content of the gas.

Water vapor plays an active role in the equilibrium of H_2S extraction so efforts will be made to determine it more precisely. It is planned to pass

the gas samples through a small bed of calcium carbide and determine the resulting acetylene produced by the action of H_2O and H_2S . A separate direct determination of H_2S will permit accurate estimates of H_2O .

Two gas chromatographs will be employed in analysis of gas samples. A Hewlett-Packard instrument equipped with a flame photometer detector will be used for determination of low concentrations of H_2S . A Carle instrument will be used to characterize the gas. This instrument employs multiple columns and a switching arrangement which prevents strongly sorbed molecules from getting beyond the first column. These can be eluted from the first column but would be irreversibly absorbed on succeeding columns.

These instruments are interfaced to the Spectra Physics integrator and printer plotter. A readout listing compounds by name and volume percent will be obtained. The Hewlett-Packard instrument (programmed for determination of sulfur compounds) has a cycle time of about 2 min/sample, so a fairly complete record of sulfur contents can be obtained.

All gases containing H_2S are corrosive. "Alonizing" eliminates corrosion of process vessels and pipe and hot gases entering sample lines will be cooled by steam tracing to $\sim 100^\circ C$ to reduce corrosion. The first part of the sample line encountered by the gas will be of Carpenter-20 tubing which is fairly corrosion resistant. The cooled gas will continue its flow through Teflon tubing on which H_2S has no effect. All gas samples will flow to a solenoid driven, 12-position valve which can be controlled remotely to select the sample which will be led to the gas chromatograph. This valve is of Kel-F, an inert plastic.

Theoretical Studies

In last quarter's report, it was stated that temperature profiles for the regenerator were obtained by arbitrarily dividing the regenerators into "N" increments of equal H_2S removal. Even with $N = 8$ actual tray temperatures would not necessarily result. The plan was to use this pseudo temperature-composition profile (at equilibrium) to zero in on actual tray temperatures.

In an improvement on this procedure, actual tray to tray enthalpy balances are used to generate the temperature profiles. In addition, the

mathematical description of the venturi, extraction column, and regeneration column as a combined system has been finalized and coded in FORTRAN-IV language.

Data which must be supplied to the computer model can be divided into two categories: 1) physical and chemical properties which remain constant for each run, and 2) experimental data.

Included in the invariant category are constants in the equilibrium expression, heat of reaction, and heat capacity coefficients for liquid and gaseous species. Also included are convergence criteria for the venturi, extractor, and regenerator routines.

Numerous options exist for specifying experimental data which may change from run to run or during a run. For clarity a single option (the most used case) will be treated here. Following two descriptor cards which give the data and a description of the run, the data shown in Table I must be input. For realistic predictions, efficiency factors (not available) should be included. Presently, estimates are used and fed in as data. When no efficiency data are read in a default case of 1.0 is used, which simply implies equilibrium is attained in all stages.

Additional data can be supplied as input information. This data is not used in the calculations but is printed out for comparison with calculated values. When no additional experimental data is supplied, fictitious numbers consisting of all nines are printed out.

1) Venturi

Calculations in the venturi require complete specification of the liquid and gas inlet streams. The subroutine then calculates the intersection point of the operating line and equilibrium curve taking efficiency into account.

Solving the operating and equilibrium curves simultaneously by algebra would be extremely difficult because of the nonlinearity of the equilibrium curve. A trial-and-error procedure is used in which a y value for the outlet gas sulfur concentration is "guessed" and a corresponding x value (MxS concentration) is calculated from the operating line equation. This x value is then

TABLE I. Required Data Inputs

For Venturi Inlet

Gas

Flow Rate (moles/hr)
Mole Fraction H_2S
Mole Fraction H_2O
Mole Fraction CO_2
Temperature in ($^{\circ}C$)

Liquid

Flow Rate (moles/hr)
Mole Fraction MxS
Temperature in ($^{\circ}C$)

For Extraction Column

Liquid

Flow Rate Out (moles/hr)
Temperature in ($^{\circ}C$)

For Regenerator

Gas

Flow Rate in (moles/hr)
Temperature in ($^{\circ}C$)
Steam/ CO_2 Ratio

Liquid

Temperature in ($^{\circ}C$)

Other

Makeup Salt

Flow Rate (moles/hr)
Mole Fraction $MxCO_3$

Bleed Stream

Flow Rate (moles/hr)
Mole Fraction MxS

used to calculate a new y value from the equilibrium expression. If this calculated y agrees with the guessed value within $\pm 0.1\%$ convergence is assumed. Pertinent mathematical relations appear in Section III-D.

2) Extractor

The extractor material balance assumes the gas inlet composition is the same as gas out the venturi. Salt composition out the extractor is calculated

from a material balance on the venturi feed tank. Measured liquid flow rate out the extractor and liquid temperature into the column are required input information.

The most used option in this subroutine is expected to be the case where isothermal column operation is assumed. In this case a bulk mixing calculation is done first to determine an "average" fluid temperature in the column. The starting point and slope of the operating line are fixed by the inlet gas and outlet liquid conditions. With temperatures now specified at each tray a stepping procedure can be started from the bottom to the top of the column. Efficiencies are used at each tray to relate equilibrium to actual compositions. Conditions at the top of the column are determined by stepping off two actual stages. These conditions represent the final gas purity out the extraction column and the salt purity required from the regenerator.

A second option allows specification of an overall recovery for H_2S . This will fix the outlet gas composition from the extractor. A simple overall material balance will then fix the inlet salt composition. No tray by tray calculations are performed under this option since it is unlikely that exactly two real stages would be needed. Establishing the inlet salt composition is necessary for the subsequent regenerator analysis. As above, details of mathematics for the extractor are deferred to Section III-D.

3) Regenerator

The primary function of this routine is to generate temperature profiles in the column. These profiles are needed to assess what operating conditions might cause temperature excursions in the column.

Inlet and outlet conditions are completely specified either as input data or from calculations in other segments of the program. Specified data are inlet gas flow rate, temperature, and steam/ CO_2 ratio plus inlet liquid temperature. Also required is heat removal rate from the top plate.

Plate-to-plate calculations then proceed as follows:

- 1) An initial linear Y profile is assumed.
- 2) Temperatures on each tray are determined by inverting the matrix of heat balance equations.

- 3) Values for the equilibrium constant are generated from the above temperatures.
- 4) With Y and K_{eq} known X_{eq} can be found.
- 5) This X_{eq} value is corrected to X_{act} using a specified tray efficiency.
- 6) The "actual" X value is used to generate a new Y value from the operating line equation.
- 7) Steps 2 through 6 are repeated until the temperature profile stabilizes, i.e., there is negligible change in any of the tray temperatures from one iteration to the next.

The routine accounts for changes in heat capacity of both liquid and gaseous materials as the tray temperatures increase or decrease. An average value for heat of reaction (between 550°C and 650°C) is used in the enthalpy balance equations. Even though compositions might not reach equilibrium values, it is assumed that thermal equilibrium is achieved. That is the liquid and gas leaving a tray are at the same temperature.

A special cutoff procedure is built into the routine. When liquid sulfur concentrations on a plate reach or go below the required outlet composition, the stepping procedure is stopped. It is then assumed that the rest of the trays in the column produce no change in either liquid or gas composition. Fluid mixing calculations are still performed, however, so tray temperatures will continue to vary.

D. Sample Outputs

Although many more cases have been run to check different aspects of the code, only three are presented (Table II), e. g.:

1) Design Conditions:

Essentially this is the baseline case for comparing all others.

2) Using Hot Fuel Gas but Cold Salt:-

Simulates the situation where the controller or heater on the venturi feed tank fails and salt temperature to the venturi drops.

**TABLE II. Molten Salt Scrubbing System
Material Balance Summary**

Gas	Venturi				Extractor				Regenerator			
	Inlet		Outlet		Inlet		Outlet		Inlet		Outlet	
	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc
Flow Moles/hr	12.540			12.649		12.649		12.698	1.470			1.312
Temp in °C	700.		700.	696.	700.	696.	700.	697.	550.		530.	595.
Comp												
M.F. H ₂ S	0.0130		0.0036	0.0043	0.0036	0.0043	0.0005	0.0004	0.0000	0.0000	0.1204	0.1207
	0.1000											
CO ₂	0.0502											
Liquid												
Flow Moles/hr	8.560			8.560		1.235	1.240	1.235		1.235	1.235	
Temp in °C	700.		700	696.	700.	700.	700.	0.	0.		600.	623.
Comp												
M.F. M _X S	0.1227		0.1363	0.1354	0.0089	0.0072	0.0419	0.0472	0.1363	0.1354	0.0089	0.0072
M.F. CO ₃	0.3310											

Fresh Salt Makeup (moles/hr) 0.000

Bleed Rate (moles/hr) 0.000

M.F. M_XS 0.000

Date: June sometime

Run No: Test Case (design conditions)

TABLE II. (Contd)

Extractor Details (Assuming an Isothermal Column)

Flows Moles/Hr	Inlet		Outlet	
	Exp	Calc	Exp	Calc
Gas		12.649		12.698
Liquid		1.235	1.240	1.235

Tray	XMS		YH2S		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Inout	Calc
Top	0.0089	0.0072			700.	700.		
2		0.0160	0.0005	0.0004	700.	697.	0.90	0.00
1		0.0472	0.0009	0.0012	700.	697.	0.90	0.00
Bot			0.0036	0.0043	700.	696.		

Regenerator Details (Using Calc I/O Comp Data)

Flows Moles/Hr	Inlet		Outlet	
	Exp	Calc	Exp	Calc
Gas	1.470			1.312
Liquid		1.235	1.235	

Tray	XMS		YHPS		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Inout	Calc
Top	0.1363	0.1354			550.	550.		
1		0.0776	0.1200	0.1207	599.	595.	0.90	0.00
2		0.0484	0.0590	0.0628	625.	619.	0.90	0.00
3		0.0318		0.0359		633.	0.90	0.00
4		0.0210	0.0160	0.0211	649.	643.	0.90	0.00
5		0.0127		0.0116		649.	0.90	0.00
6		0.0072	0.0063	0.0046	652.	651.	0.90	0.00
7		0.0072		0.0046		645.	0.90	0.00
8		0.0072	0.0063	0.0046	621.	623.	0.90	0.00
Bot			0.0000	0.0000	550.	550.		

Date: June sometime

Run No: Test Case (design conditions)

TABLE II. (Contd)

Gas	Venturi				Extractor				Regenerator			
	inlet		Outlet		inlet		Outlet		Inlet		Outlet	
	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc
Flow Moles/hr	12.540			12.505		12.605		12.684	1.470			1.326
Temp in °C	700.		700.	532.	700.	532.	700.	647.	550.		580.	597.
Comp												
M.F. H ₂ S	0.0130		0.0036	0.0078	0.0036	0.0078	0.0005	.0015	0.0000	0.0000	0.1204	0.1089
H ₂ O	0.1000											
CO ₂	0.0502											
Liquid												
Flow Moles/hr	8.560			8.560		1.235	1.240	1.235		1.235	1.235	
Temp in °C	600.		700.	632.	700.	700.	700.	3.	550.		600.	616.
Comp												
M.F. M _x S	0.1227		0.1363	0.1302	0.0089	0.0134	0.0419	0.0779	0.1363	0.1302	0.0089	0.0134
M.F. CO ₃	0.3310											

Fresh Salt Makeup (moles/hr) 0.000

Bleed Rate (moles/hr) 0.000

M.F. M_xS 0.0000

Date: June sometime

Run No: Using Hot Syn Gas But Cold Salt

TABLE II. (Contd)

Extractor Details (Assuming an Isothermal Column)

Flows Moles/hr		Inlet		Outlet	
		Exp	Calc	Exp	Calc
Gas			12.605		12.684
Liquid			1.235	1.249	1.235

Tray	XMS		YH2S		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Input	Calc
Top	0.0089	0.0134			700.	700.		
2		0.0349	9.0005	0.0015	700.	647.	0.90	0.00
1		0.0779	0.0003	0.0036	700.	647.	0.90	0.00
Bot			0.0036	0.0078	700.	632.		

Regenerator Details (Using Calc I/O Comp Data)

Flows Moles/hr		Inlet		Outlet	
		Exp	Calc	Exp	Calc
Gas			1.470		1.326
Liquid			1.235		1.235

Tray	XMS		YH2S		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Input	Calc
Top	0.1363	0.1302			550.	550.		
1		0.0705	0.1200	0.1089	599.	597.	0.90	0.00
2		0.0403	0.0590	0.0505	625.	622.	0.90	0.00
3		0.0219		0.0231		636.	0.90	0.00
4		0.0134	0.0160	0.0072	649.	642.	0.90	0.00
5		0.0134		0.0072		642.	0.90	0.00
6		0.0134	0.0063	0.0072	652.	640.	0.90	0.00
7		0.0134		0.0072		635.	0.90	0.00
8		0.0134	0.0063	0.0072	621.	616.	0.90	0.00
Bot			0.0000	0.0000	550.	550.		

TABLE II. (Contd)

Date: June Sometime

Run No: Using Cold Syn Gas but Hot Salt

Gas	Venturi				Extractor				Regenerator			
	Inlet		Outlet		Inlet		Outlet		Inlet		Outlet	
	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc	Exp	Calc
Flow Moles/hr	12.540			12.615		12.615		12.690	1.470			1.320
Temp in °C	550.		700.	647.	700.	647.	700.	659.	550.		580.	596.
Comp												
M.F. H ₂ S	0.0130		0.0036	0.0069	0.0036	0.0069	0.0005	0.0010	0.0000	0.0000	0.1204	0.1136
CO ₂	0.0502											
Liquid												
Flow Moles/hr	8.560			8.560		1.235	1.240	1.235		1.235		1.235
Temp in °C	700.		700.	647.	700.	700.	700.	0.	550.		600.	619.
Comp												
M.F. M _x S	0.1227		0.1363	0.1315	0.0089	0.0101	0.0419	0.0705	0.1363	0.1315	0.0089	0.0101
M.F. CO ₃	0.3310											

Fresh Salt Makeup (Moles/hr) 0.000

Bleed Rate (Moles/hr) 0.000

M.F. M_xS 0.0000

TABLE II. (Contd)

Date: June Sometime

Run No. Using Cold Syn Gas but Hot Salt

Extractor Details (Assuming an Isothermal Column)								
Flows Moles/hr		Inlet		Outlet				
		Exp	Calc			Exp	Calc	
Gas			12.615				12.690	
Liquid			1.235		1.240		1.235	
Tray	XMS		YH2S		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Input	Calc
Top	0.0089	0.0101			700.	700.		
2		0.0283	0.0005	0.0010	700.	659.	0.90	0.00
1		0.0705	0.0009	0.0028	700.	659.	0.90	0.00
Bot			0.0036	0.0069	700.	647.		
Regenerator Details (Using Calc I/O Coma Data)								
Flows Moles/hr		Inlet		Outlet				
		Exp	Calc			Exp	Calc	
Gas			1.470				1.320	
Liquid			1.235				1.235	
Tray	XMS		YH2S		Temp °C		Efficiency	
	Exp	Calc	Exp	Calc	Exp	Calc	Input	Calc
Top	0.1363	0.1315			550.	550.		
1		0.0729	0.1200	0.1136	599.	596.	0.90	0.00
2		0.0435	0.0590	0.0557	625.	621.	0.90	0.00
3		0.0263		0.0288		635.	0.90	0.00
4		0.0143	0.0160	0.0137	649.	644.	0.90	0.00
5		0.0101		0.0035		646.	0.90	0.00
6		0.0101	0.0063	0.0035	652.	645.	0.90	0.00
7		0.0101		0.0035		639.	0.90	0.00
8		0.0101	0.0063	0.0035	621.	619.	0.90	0.00
Bot			0.0000	0.0000	550.	550.		

3) Using Cold Fuel Gas but Hot Salt:

Simulates the situation where the gas preheater may have failed and fuel gas enters at a lower temperature than the salt.

1. Design Conditions and General Comments

Most portions of the Material Balance Summary (Table II) should be self-explanatory. For data points with both calculated and experimental values shown the "experimental" values are for now the hand calculated ones generated during design. They are not used in calculations but merely printed out for easy visual comparison. The small differences seen in mole fraction values can be attributed to differences in temperatures used in calculations. Design calculations assumed an isothermal venturi and extraction column whereas the computer model takes into account the actual slight temperature effects. Another difference lies in stages used for calculations. Both the extractor and regenerator have been oversized to provide safety margins. The safety margins were needed to compensate for uncertainties in physical and chemical properties of the system which were used in the calculations.

The Extractor Details and Regenerator Details section again follow the same ideas as in the Summary section. Notice the extractor operates isothermally but the temperature lies between that of the liquid feed and gas feed.

In both the extractor and regenerator sections, blanks in the EXP columns indicate that no experimental data will be available at those points, e.g., only every other tray in the regenerator can be sampled for gas composition or measured for temperature. The zeros in the EFFICIENCY/CALC column imply no efficiencies have been calculated, hence only input values are used in the program. The TOP and BOTTOM lines show liquid entering the top of each column and gas entering the bottom of each vessel.

For the regenerator column printed liquid and gas compositions do not change on the bottom three trays. This is simply an indication that the required liquid purity has been reached and the other trays are not needed for the desired separation. In the actual system, some changes will be expected on all trays but the changes should be very small in the bottom of the column.

2. Using Hot Fuel Gas but Cold Salt

Here the salt temperature to the venturi has arbitrarily been dropped to 600°C. This results in a much "dirtier" gas stream out the venturi. Salt to the extractor is assumed to be heated back up to 700°C, however, the gases entering are still cold (632°C). The combination of cold and dirty gas is too much for the extractor and the exit gas composition does not have desired purity.

The calculation procedure uses the extractor gas outlet composition to determine required liquid purity from the regenerator. Hence for this case the regenerator needs to supply only a relatively dirty salt. It can do this with only three actual stages. Since purity requirements are less stringent the load on the regenerator is less and temperature excursions are less severe than in the design case.

3. Using Cold Fuel Gas but Hot Salt

For this example the temperature of gas into the venturi has been dropped to 550°C. Changes from design conditions are fairly slight. The reason for this is that the liquid has a much higher thermal mass than the gas stream. Hence temperature drops in the venturi and extractor are less severe than in the cold salt case.

E. Mathematical Detail

<u>Major</u>	<u>Symbols</u>	
a	Activities	
B,E	Known Constants in Expression for K_{eq}	
C_p	Heat Capacity	Btu/# mole/hr
G	Gas Flow Rate	# mole/hr
ΔH_r	Heat of Reaction	Btu/# mole
K_{eq}	Equilibrium Constant	
L	Liquid Flow Rate	# mole/hr
ΔM	Change in Moles of Something	# mole/hr
P	Total Pressure	ATM
T	Temp °C	°C
TA	Temp °K	°K
X	Mole Fraction M_{xS} in Liquid	

Y Mole Fraction H_2S in Gas
 η Efficiency

Subscripts

In, Out, Avg	Self Explanatory
H_2S , H_2O , CO_2 , M_x , CO_3 , M_x^s	Self Explanatory
Ex	Extractor
Ven	Venturi
i	Tray i
G	Gas
L	Liquid
Rcy	Recycle

Superscripts

* Equilibrium Value

1. PERTINENT EQUATIONS FOR THE VENTURI

Chemical Reaction

Material Balance

$$G_{in} Y_{in} - G_{out} Y_{out} = L_{out} - L_{in} X_{in}$$

where $G_{out} = \frac{G_{in} (1 + Y_{in})}{(1 - Y_{out})}$ because of chemical reaction taking place.

Equilibrium

$$K_{eq} = \text{EXP} (B - E/TA)$$

$$= \frac{A_{M_xS} A_{H_2O} A_{CO_2}}{A_{M_xCO_3} A_{H_2S}} \text{ in terms of activities.}$$

$$= \frac{X_{M_xS}}{X_{M_xCO_3}} \cdot \frac{Y_{H_2O} Y_{CO_2}}{Y_{H_2S}} \cdot P \quad \text{The approximation used in calculations.}$$

Enthalpy Balance (Assumes property changes are small enough that averages can be used)

$$\Delta M = \text{moles } H_2S \text{ reacting/hr} = G_{out} Y_{out} - G_{in} Y_{in}$$

$$G_{avg} C_{p_{avg_g}} (T_{out} - T_{in_g}) = L C_{p_{avg_l}} (T_{in_l} - T_{out}) - \Delta m \Delta H_r$$

Note T_{out} is assumed the same for both the liquid and gas streams, but inlet temperatures can be different.

Efficiency

$$\eta_v = \frac{Y_{in} - Y_{out}}{Y_{in}} \quad \text{This is not a true efficiency but is ratio of actual sulfur removed to total sulfur present.}$$

2. PERTINENT EQUATIONS FOR THE EXTRACTOR

Material Balance

At venturi feed tank:

$$L_{out_{Ex}} + L_{Rcy} = L_{in_{Ven}} + L_{bleed}$$

or

$$L_{out_{Ex}} X_{out_{Ex}} + L_{Rcy} X_{out_{Ven}} = L_{in_{Ven}} X_{in_{Ven}} + L_{Bleed} X_{Bleed}.$$

Inside absorber (from bottom to tray i)

$$(L_{i+1} X_{i+1} - L_{out} X_{out}) = G_i Y_i - G_{in} Y_{in}.$$

Where L is constant

$$G_i = \frac{G_{in} (1 + Y_{in})}{(1 + Y_i)}$$

Equilibrium

(See venturi section--same relationship holds).

Enthalpy Balance

(Really a bulk mixing calculation to get an approximate average temperature in the column--heat of reaction is ignored).

$$G_{in} * C_{p_g} * (T_{in_g} - T_{avg}) = L * C_{p_L} (T_{avg} - T_{in_L})$$

Efficiency

$$\eta_i = \frac{Y_i - Y_{i-1}}{Y^* - Y_{i-1}} = \frac{\text{actual change}}{\text{change if equation had been achieved}}$$

3. PERTINENT EQUATIONS FOR THE REGENERATOR

Material Balance (between * top of column and tray i)

$$G_{i+1} Y_{i+1} - G_{out} Y_{out} = L(X_i - X_{in})$$

where

$$G_{out} = G_{in} / (1 + Y_{out})$$

$$G_{in} = G_{in} (1 + Y_{in})$$

also

$$AM = \text{moles } H_2S \text{ liberated/hr} = L (X_{in} - X_{out}).$$

Equilibrium

Equilibrium constants are based on reverse reaction (see more detail in venturi section), i.e.:

$$K_{eq_i} = \exp(B - E/TA_i)$$

$$= \frac{X_{M_x S_i}}{X_{M_x CO_3_i}} \cdot \frac{Y_{H_2O_i} Y_{CO_2_i}}{Y_{H_2S_i}} P.$$

Efficiency

$$E_i = \frac{X_i - X_{i-1}}{X_i^* - X_{i-1}} = \frac{\text{actual liquid composition change}}{\text{change if equilibrium had occurred}}$$

Heat Balance Equations (from bottom of column to tray i)

$$L C_{pL} (T_L - 1 - T_n) = G_{av} C_{pg} (T_i - T_{n+i}) + G_i Y_i \Delta H_r$$

where

$$G_{av} = (G_{in} + \frac{G_{in}}{1 + Y_i}) / 2$$
$$G_i = \frac{G_{in}}{1 + Y_i}$$

Note: Tray 1 is actually at the top of the column.

E. PROGRAM MANAGEMENT

Task descriptions defined in the precedence diagram of last quarter's report remain unchanged. A schedule slippage of 4 to 6 wk must be accepted, however, due to delays in receipt of "Alonized" pipe and equipment from Alon Processing, Inc. Tasks defined by cross-hatched areas are critical path items and cannot be completed until this material is received. Many supplemental tasks must also be deferred. This will delay completion of the PDU until late in September.

IV. PROPOSED WORK DURING THE NEXT QUARTER

All construction should be completed by the end of the next quarter. Individual equipment items such as air preheat and CO₂-steam preheat systems should have been test operated. All pipe should be leak tested cold as well as hot and the plant readied for test runs. All materials should be on hand.

V. OVERALL PROJECT STATUS

Procurement of materials and equipment is nearly complete with delivery on a few key items pending within a matter of days. Coal will be ordered soon, the timing here being keyed to plant completion because of the instability of noncaking coals (tendency to slack). Plant completion is anticipated by the end of September.

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