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## PROCESS FEASIBILITY STUDY IN SUPPORT OF SILICON MATERIAL TASK I

QUARTERLY TECHNICAL PROGRESS REPORT (VIII)

September, 1977

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CALIFORNIA INSTITUTE OF TECHNOLOGY JET PROPULSION LABORATORY (JPL) 4800 Oak Grove Drive Pasadena, California 91103

Approval Signature Carl 2. You

#### Technical Content Statement

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#### ABSTRACT

Major activities during this reporting period were focused on process system properties, chemical engineering and economic analyses.

In Task 1, analyses of process system properties were continued for silicon course materials under consideration for solar cell grade silicon including data collection, analysis, estimation and correlation.

Initial correlation efforts focused on vapor pressure data which are extremely important in phase equilibria in a chemical plant processing silicon source materials. The vapor pressure of silicon tetrachloride as a function of temperature was correlated by the relation

$$\log P_{v} = A + \frac{B}{T} + C \log T + DT + ET^{2}$$

Values for the correlation constants A,B,C,D and E are presented. The versatile correlation covers both low and high pressure regions. The agreement of correlation and data values is good with average absolute deviation of only 0.7% for fifty-eight data points tested.

Correlation results for gas phase heat capacity of silicon tetrachloride

$$C_{p} = A + BT + CT^{2} + DT^{3}$$

are presented including data from American, Russian, German and Japanese sources.

The apparatus for measuring thermal conductivity of gases was assembled and calibrated. This included the determination of cell constants and filament wire temperatures. The accuracy of data to be obtained with this equipment was evaluated by measuring the thermal conductivity of argon in the temperature range 25°C to 400°C. Comparison of measured data in this study with recommended values from the literature was favorable with small deviations of only  $\pm 2$ % up to 300°C and  $\pm 4$ % above 300°C.

Chemical engineering analysis in Task 2 was continued on the silane process (Union Carbide) using the revised flowsheet from Mr. W.C. Breneman. Material balance is about 95% complete for the preliminary design. Energy balance, property data and equipment design are about 60% complete.

The review and modification of the preliminary process design for the conventional polysilicon process were completed, and results are presented. Design criteria were selected so that results would be comparable to alternate processes under consideration. Major modifications and key items are reviewed. For Task 3, cost analysis activities for the production of semiconductor grade polysilicon via the conventional hair pin process technology were continued. Three cases (Case A, B, and C) were considered with results summarized below for low and high electrical costs:

- 1. Case A
   . Product Cost (Sales Price).....63.6-70.3\$/KG Si@ 10% ROI
- 2. Case B
  . Product Cost (Sales Price).....61.1-67.7\$/KG Si @ 25% ROI
- 3. Case C
   . Product Cost (Sales Price).....64.8-72.7\$/KG Si @ 25% ROI

Case C probably best represents the current situation for polysilicon production of semiconductor grade. It is based on current 1977 costs (raw materials, labor, utilities, etc.) for a polyplant constructed in the 1960's. Many polyplants in the U.S.A. were constructed in 1960 or earlier and are producing polysilicon at current operating costs (labor, utilities, etc.). The product cost (sales price) of 64.8-72.7\$/KG Si includes a profit of 25% ROI (return on investment).

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#### I. PROCESS SYSTEM PROPERTIES ANALYSES (TASK 1)

#### A. SILICON TETRACHLORIDE PROPERTIES

Major efforts were continued on process system properties of silicon source materials under consideration for solar cell grade silicon production including data collection, analysis, estimation and correlation for properties required in the performance of the chemical engineering analyses of the alternate processes.

Initial correlation activities focused on vapor pressure data for silicon tetrachloride. Vapor pressure data for pure components such as silicon tetrachloride and additional silicon source materials are extremely important in phase equilibria in a chemical plant processing such materials. Most dew point, bubble point and flash calculations in mass transfer operations (such as distillation) involve knowledge of the vapor pressure of the respective pure components. Engineering design of pressure requirements for storage equipment and various process vessels require knowledge of the vapor pressure of the components being stored or processed.

The vapor pressure of silicon tetrachloride as a function of temperature was based on the following correlation relation:

$$\log P_{V} = A + \frac{B}{T} + C \log T + DT + ET^{2}$$
 IA-1)

where

P. = vapor pressure of saturated liquid, mm of Hg

A, B, C, D, E = correlation constants for chemical compound

 $T = temperature, ^{\circ}K$ 

The correlation constants (A, B, C, D and E) were determined using a generalized least squares computer program for minimizing deviation of calculated and experimental data values screened from the literature. Average absolute deviation was about 0.7% for the fifty-eight data points.

In processing the data points, various other vapor pressure equations were evaluated. The above equation was selected based on better agreement with experimental data. Greater deviations were encountered with the other vapor pressure equations.

The correlation constants (A, B, C, D and E) are presented in Table IA-1. The table also presents the experimental data and calculated value at each temperature level. The last column gives the difference between the experimental and calculated values on a percentage basis, (cal-exp)/exp, which is the percent error. In most cases, the error is quite small (less than 1%) at both low and high pressures. The vapor pressure of silicon tetrachloride at any temperature in the region of the triple point and up to the critical point may be calculated with the correlation constants presented. Both low and high pressure regions are covered by the unique correlation. The value for the acentric factor ( $\omega$ ) is also given in Table IA-1. The acentric factor which is defined by

$$\omega = -\log P_r - 1.000$$
 (at  $T_r = 0.70$ ) (IA-2)

where  $P_{r}$  = reduced pressure,  $P_{r}/P_{c}$ 

 $T_{r}$  = reduced temperature  $T/T_{r}$ 

is an important parameter in generalized thermodynamic correlations involving virial coefficients, compressibility factor, enthalpy and fugacity.

Correlation and data values are compared in Figure IA-1 for silicon tetrachloride. The agreement is quite good as shown in the computer plot.

These results - correlation constants for vapor pressure - will be utilized in the performance of the chemical engineering analysis for those processes using silicon tetrachloride such as the silane process (Union Carbide).

Heat capacity data for silicon tetrachloride as ideal gas at low pressure are available from American, Russian, German and Japanese souces (B10, B17, B20, B34, B76 and B84). The values, which are primarily based on structural and spectral measurements, are in close agreement. Differences among the sources are about 1.2% or less.

The heat capacity data for the gas phase were correlated by a series expansion in temperature:

$$C_{p} = A + BT + CT^{2} + DT^{3}$$
 (IA-1)

where C = heat capacity of ideal gas at low pressure, cal/(g-mol) (°K); A, B, C<sup>P</sup> and D = characteristic constants for the chemical compound; and T = temperature, °K.

The correlation constants were determined from a least-squares fit of the available data. The numerous data points were processed with a generalized least-squares computer program for minimizing the deviation.

The correlation constants (A, B, C and D) for gas heat capacity are given in Table IA-2. The table also shows the agreement of the experimental and calculated values at each temperature level. The deviation in most cases is quite small (less the 1%) at both low and high temperatures. Average absolute deviation is about 0.7% for the fifty-two data points.

For silicon tetrachloride, heat capacity of the gas versus temperature is shown in the computer plot of Figure IA-2. Both correlation and data values are presented in the plot.

These results - correlation constants for gas phase heat capacity - will be utilized in the performance of the chemical engineering analysis for those processes using silicon tetrachloride. TABLE IA-1 CORRELATION CONSTANTS FOR VAPOR PRESSURE OF SILICON TETRACHLORIDE SILICON TETRACHLORIDE CRIT\_TEMP (DEG\_C) 234.000 MOLEC WT 169.900 -69.400 CRIT PRESS (ATM) 37.000 MELT PT (DEG C) CRIT VOL (CC/G MOL) 326,300 BOIL PT (DEG C) 57.300 CRIT COMP FACT (ZC) 0.290 0.2556 CALCULATED ACCENTRIC FACTOR LOG PV = A + B/T + CLOG(T) + DT + ET2FOR VAPOR PRESSURE - PV WHERE PV IS IN MM MERCURY AND T IS IN DEG K A = 0.74284129E 01 B = -0.20398218E 04 C = 0.21658116E 01WHERE E = 0.11877907E - 04D=-0.15519367E-01 FOR THE TEMPERATURE RANGE OF -63.40 TO 234.00 DEG C

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REF	TEMP (DEG C)	EXP	CALC	CALC-EXP	PCT ERROR
85	0.	77.0000	76.6922	0.3078	0.399736
37	0.55	78,2000	78.8289	-0,6289	-0.804235
3.4	5.28	98.7000	99.3151	-0.6151	-0.623151
	12.37	136.5000	138.0503	-1,5503	-1.135772
	19.82	189,5000	191.2044	-1.7044	-0.899399
	29.53	281.6000	284.1311	-2.5311	-0.898811
	34.41	340.2000	342.8654	-2.6654	-0.783482
	40.32	423.4000	426.5173	-3,1173	-0.736253
	52.53	645,4000	650.1748	-4.7748	-0.739823
B7	2.20	86.3000	85.5361	0.7639	0.885212
	25.10	239.0000	238.0605	0,9395	0.393086
	34.20	340,7000	340.1537	0.5463	0.160342
	40.60	431.7000	430.8478	0.3522	0.197400
	46.50	531,0000	530.4765	0,5235	0.098590
	56.90	752,2000	749.3905	2.8095	0.373500
324	-35.10	10,0000	9.6819	0.3131	3.181341
	-24.40	20.0000	19.5744	0.4256	2.127987
	-12.60	40 <u>.000</u> 0	39.3450	0.6550	1.637443
	-5.00	60.0000	59.3727	0.6273	1.045476
	5.30	100.0000	99.4101	0,5899	0.589859
	20.90	200.0000	200.1240	-0.1240	-0.061991
	38.60	400.0000	400.6651	-0.6651	-0.166263
	<b>57.3</b> 0	760.0000	759.0293	0.9707	0.127718
827	0.	77.0000	76.6922	0.3078	0.399736
	5.00	98.0000	97.9916	0.0084	0.008611
	10.00	124.0000	123.9298	0.0702	0.056651
	15.00	153,0000	155.2278	-2.2278	-1.456051
	20.00	191.0000	192.6682	-1.6682	-0.873407
	25.00	235,0000	237.0947	-2.0947	-0.891346
	30.00	287.0000	289,4103	-2.4103	-0.839810
	35.00	346.0000	350.5762	-4.5762	-1.322612
	40.00	419.0000	421.6103	-2.6103	-0.622974
	45.00	501.0000	503.5843	-2.5843	-0.515825
	50.00	599.0000	· 597.6227	1.3773	0.229942
	55.00	709,0000	704.9005	4.0995	0.578204
	60.00	839.0000	826.6418	12.3582	1.472969
B30	-34.40	10.0000	10.1612	-0,1612	-1.611549

# TABLE IA-1 (continued)

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	5.00	100,0000	97.9916	2.0084	2.008439
	38.40	400,0000	397.7415	2.2585	0.564619
B32	-63.36	1,0000	1.0027	-0.0027	-0.268468
	-34.56	10,0000	10.0498	-0.0498	-0.498466
	5.34	100.0000	99.6006	0.3994	0.399439
	57.34	760,0000	759.9985	0.0015	0.000192
352	-63.40	1.0000	0.9990	0.0010	0,103006
-	-44.10	5,0000	5.0441	-0.0441	-0.881665
	-34.40	10,0000	10.1612	-9,1612	-1.611549
	-24.00	20,0000	20.0688	-0.0688	-0.344111
	-12.10	40.0000	40.4599	-0.4599	-1.149820
	-4.80	60,0000	59.9968	0.0032	0.005365
	5.40	100.0000	99•8868	0.1132	0.113250
	21.00	200,0000	200.9666	-0,9566	-0.483283
	38.40	400,0000	397.7415	2.2585	0.564619
	56.80	760.0000	746.9957	13.0043	1.711086
878	20.00	192.6000	192.6682	-0.0682	-0.035414
	30.00	289,8000	289.4103	0.3397	0.134487
	40.00	422,6000	421.6103	0,9897	0.234202
	50.00	599.5000	597.6227	1.8773	0.313153
CRIT	234.00	28120.0000	28153.2566	-33.2566	-0.118267
	NUMBER C	OF POINTS	58		
	RMS ERRO		5,2276		
		ABS ERROR	2,1318		
		EXP VALUE	748,6362		
		PCT ERROR	0,6981		

SILICON TETRACHLORIDE

169.900 CRIT TEMP (DEG C) 234.000 MOLEC WT CRIT PRESS (ATM) 37.000 MELT PT (DEG C) -69.400 CRIT VOL BOIL PT (DEG C) 57.300 (CC/G MOL) 326.300 0.290 CRIT COMP FACT (ZC) CALCULATED ACCENTRIC FACTOR 0.2556 LOG PV = A + B/T + CLOG(T) + DT + ET2FOR VAPOR PRESSURE - PV WHERE PV IS IN MM MERCURY AND T IS IN DEG K B=-0.20398218E 04 C= 0.21658116E 01 A= 0.74284129E 01 WHERE E= 0.11877907E-04 D = -0.15519367E = 01FOR THE TEMPERATURE RANGE OF -63.40 TO 234.00 DEG C

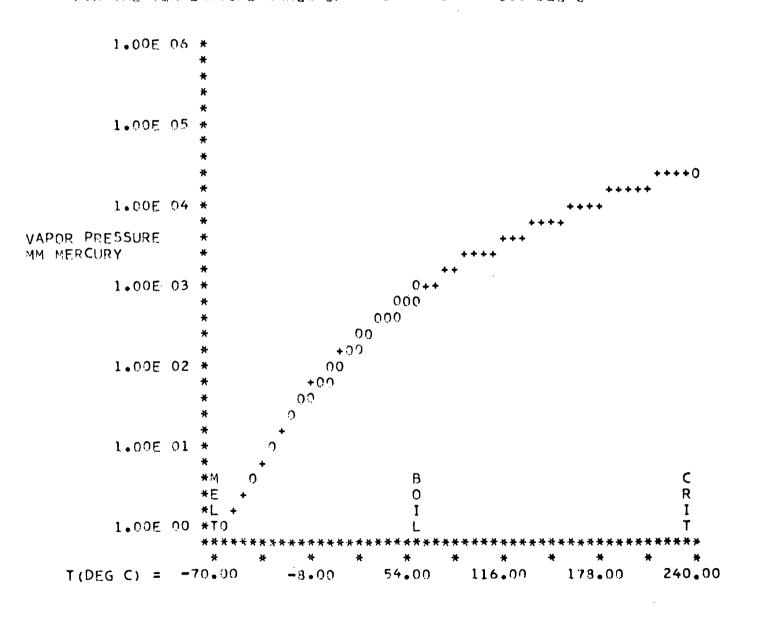


FIGURE IA-1 VAPOR PRESSURE OF SILICON TETRACHLORIDE VS. TEMPERATURE ( O DATA, + CORRELATION )

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TABLE IA-2

CORRELATION CONSTANTS FOR HEAT CAPACITY (GAS) OF SILICON TETRACHLORIDE SILICON TETRACHLORIDE

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MOLEC WT MELT PT (DEG BOIL PT (DEG		CRIT TEMP (DEG C)       234.000         CRIT PRESS (ATM)       37.000         CRIT VOL (CC/G MOL)       326.300         CRIT COMP FACT (ZC)       0.290
FOR GAS HEAT	CAPACITY - CP	CP(G) = À + BT + CT2 + DT3 WHERE CP IS IN CAL/G MOLE DEG K AND T IS IN DEG K
	0.16295843E 02 0.56611800E-08	B= 0.23530542E-01 C=-0.20046636E-04
FOR THE TEMP	ERATURE RANGE OF	0. TO 1326.84 DEG C

REF	TEMP (DEG C)	EXP	CALC	CALC-EXP	PCT ERROR
B10	25.00	21.6300	21.6796	-0.0496	-0.229462
	26.84	21.6700	21.7037	-0.0337	-0.155332
	126.84	23.1800	22.8629	0.3171	1.367931
	226.84	24.0200	23.7571	0.2629	1.094492
	326.84	24,5300	24.4202	0,1098	0.447639
	426.84	24.3600	24.8862	-0.0262	-0.105211
	526.84	25.0700	25.1890	-0.1190	-0.474487
	626.84	25,2300	25.3626	-0.1326	-0.525389
	726.84	25,3400	25.4409	-0.1009	-0.399299
317	826.84	25,4200	25.4580	-0.0380	-0.149646
	926.84	25,4900	25.4479	0.0421	0.165333
	1026.84	25,5400	25.4443	0.0957	0.374530
	1126.84	25,5300	25.4315	0.0985	0.385173
	1226.84	25,6109	25.5932	0.0168	0.065572
<b>B20</b>	0.	21.1400	21.3430	-0.2030	-0.960387
	10.00	21,3600	21.4799	-0.1200	-0.561564
	20.00	21.5800	21.6138	-0.0338	-0.156751
	30.00	21.7800	21.7447	0.0353	0.162124
	40.00	21,9700	21.8726	0.0974	0,443454
	50.00	22,1500	21.9975	0.1525	0.688440
	60.00	22,3200	22.1195	0.2005	0.898132
	70.00	22.4700	22.2387	0.2313	1.029438
	80.00	22.6300	22.3550	0.2750	1,215245
	90.00	22.7600	22.4685	0,2915	1.280821
	100.00	22.8900	22.5792	0.3108	1.357780
	200.00	23.8700	23.5412	0.3288	1.377453
	300.00	24.4300	24.2630	0.1670	0.683648
B28	56.74	22.0000	22.0801	-0.0301	-0.363974
834	24.84	21,6300	21.6775	-0.0475	-0.219779
	126.84	23.1900	22.8629	0.3271	1.410463
	226.84	23,3700	23.7571	-0.3371	-1.656410
	326.84	24.4700	24.4202	0.0498	0.203539
	426.84	24.8400	24.8862	-0.0462	-0.185811
	526.84	25.1400	25.1890	-0.0490	-0.194725
	626.84	25.4000	25.3626	0.0374	0.147419
	726.84	25.6400	25.4409	0.1991	0.776409
876	24.99	21.5700	21.6795	-0.1095	-0.507658
B84	1326.84	25.6320	25.8135	-0,1815	-0,708159
	1226.84	25.6040	25,5932	0.0108	0.042154

# TABLE IA-2 (Continued)

24.84	21.5730	21.6775	-0.1045	-0.484580
26.84	21.6100	21.7037	-0.0937	-0.433413
126.84	21.1332	22.8629	-1.7299	-8.185841
226.84	23,9840	23.7571	0,2269	0.946035
326.84	24.5050	24.4202	0.0848	0.346076
426.84	24.8350	24.8862	-0.0512	-0.205981
526.84	25.0570	25.1890	-0.1320	-0.526615
626.84	25.2140	25.3626	-0.1486	-0.589180
726.84	25.3290	25.4409	-0.1129	-0.445866
826.84	25.4130	25.4580	-0.0450	-0.177232
926.84	25.4790	25.4479	0.0311	0.122232
1026.84	25.5300	25.4443	0.0957	0.335507
1126.84	25,5710	25.4915	0.0895	0.350113
NUMBER OF	F POINTS	52		
		0 2086		

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NUMBER OF PUINIS	54
RMS ERROR	0,2886
AVERAGE ABS ERROR	0.1606
AVERAGE EXP VALUE	23.8123
AVE ABS PCT ERROR	0.6984

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# SILICON TETRACHLORIDE

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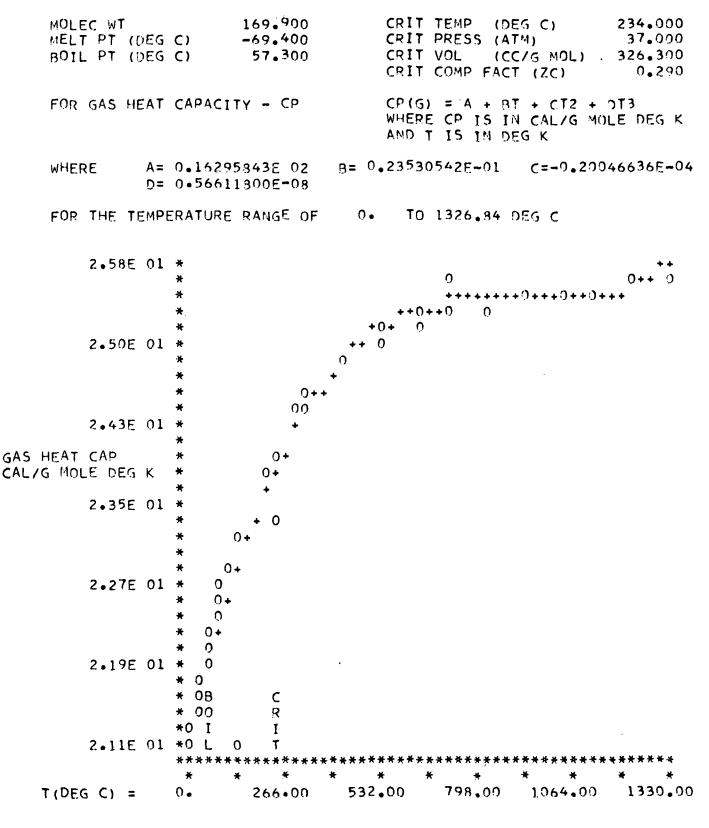


FIGURE IA-2 HEAT CAPACITY (GAS) OF SILICON TETRACHLORIDE VS. TEMPERATURE (O DATA, + CORRELATION)

#### B. THERMAL CONDUCTIVITY INVESTIGATION

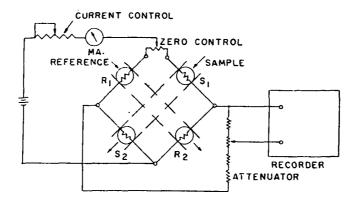
During this reporting period, preparations were begun to experimentally determine gas thermal conductivities in the temperature range 30°C to 400°C. The necessary apparatus has been assembled and calibration of the instrument has been initiated.

The apparatus to be used is a hot wire thermal conductivity cell (or catharometer). It consists of two pairs of matched tungsten-rhenium filaments mounted in a stainless steel block. The filaments are connected as elements of a constant current Wheatstone Bridge (Figure IB-1). The cell is electrically heated and a constant temperature is maintained with a digital temperature controller and read-out to ± 1°C. The filaments are positioned in cavities in the steel block into which the gases, of which the thermal conductivity is to be determined, can be introduced. The filaments are heated by a constant current and the heat thus generated is dissipated primarily by conduction through the gas. A change in the thermal conductivity of the gaseous medium results in a change in the rate of dissipation and therefore, a change in the temperature of the filament. The temperature of the hot filament is measured as if it were a resistance thermometer; change in temperature produces a change in filament resistance, which is measured by means of the Wheatstone Bridge circuit.

Since absolute measurement of thermal conductivity is difficult, a differential method will be employed where the catharometer is divided into two parts where half of the filaments are in contact with a reference gas of known thermal conductivity and the other half contact the sample whose thermal conductivity is to be determined. The Wheatstone Bridge is first balanced by introducing the reference gas into both sides of the cell. The sample to be determined is then introduced into the sample side of the cell and the resultant voltage unbalance (E) is recorded. The catharometer responds to the reciprocal of the thermal conductivities according to equation IB-1:

$$E - E_{ref.} = b(\frac{1}{\lambda} - \frac{1}{\lambda ref})$$
(IB-1)

where  $E_{ref}$  is voltage with the reference gas in both sides of the thermal conductivity cell,  $\lambda$  and  $\lambda_{ref}$  are the thermal conductivities of the unknown and reference gas respectively, and b is a constant characteristic of the particular apparatus (cell constant). This cell constant (b) can be determined by using a standardization gas of known thermal conductivity as the sample and determining the voltage unbalance (E) of it with respect to the reference gas. The cell constant (b) is slightly temperature dependent and must be determined throughout the temperature range in which measurements are to be made.



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Figure IB-1 Wheatstone Bridge Circuit For Thermal Conductivity Cell

Calibration studies were initiated on the thermal conductivity apparatus which was set-up and described. The calibration work has included the determination of cell constants for the temperature range 25°C to 400°C, the determination of filament wire temperatures for various filament currents and cell wall temperatures, and the experimental determination of the thermal conductivity of argon in the temperature range 25°C to 400°C.

The cell constant, which is used to calculate thermal conductivity values when the differential method is used, is temperature dependent and therefore needs to be determined for the complete temperature range to be investigated. It was also found that at a given temperature, the cell constant may vary slightly from day to day; therefore cell constants will be routinely determined everytime data is collected. This variation may be due to slight changes in the filament current or to slight oxidation or corrosion of the filament with use.

In measuring the thermal conductivity of gases using the "hot wire" method, the gas may not be at a uniform temperature due to differences in the temperature of the cell wall and filament wire. This can be minimized by operating the apparatus at filament currents sufficiently low that this temperature difference is small. In order to do this, a means of monitoring the filament wire temperature was needed. This was accomplished by using the filament as a resistance thermometer. With no current in the filament, the filament resistance as a function of temperature was measured (figure IB-2). When thermal conductivity data is being obtained, the filament resistance will be routinely calculated by monitoring the current through the filament and the potential across the filament. The filament temperature can then be obtained from figure IB-1. The filament current can then be adjusted so that the temperature difference between the filament and the cell wall will be small.

The thermal conductivity of argon was determined through out the temperature range 25°C to 400°C. These values were compared to recommended values for the thermal conductivity of argon(reference 36) in order to evaluate the accuracy of data obtained on this apparatus (figure IB-3). The recommended values used were those presented in "Thermophysical Properties of Matter", Vol.3 on Thermal Conductivity (TPRC), and were determined by an evaluation of available published data. It was stated that the published data correlated with the recommended values to within  $\frac{1}{2}$ %. The thermal conductivity values obtained in this study agree with the recommended values to within  $\frac{1}{2}$ % up to 300°C and  $\frac{1}{2}$ % from 300°C to 400°C.

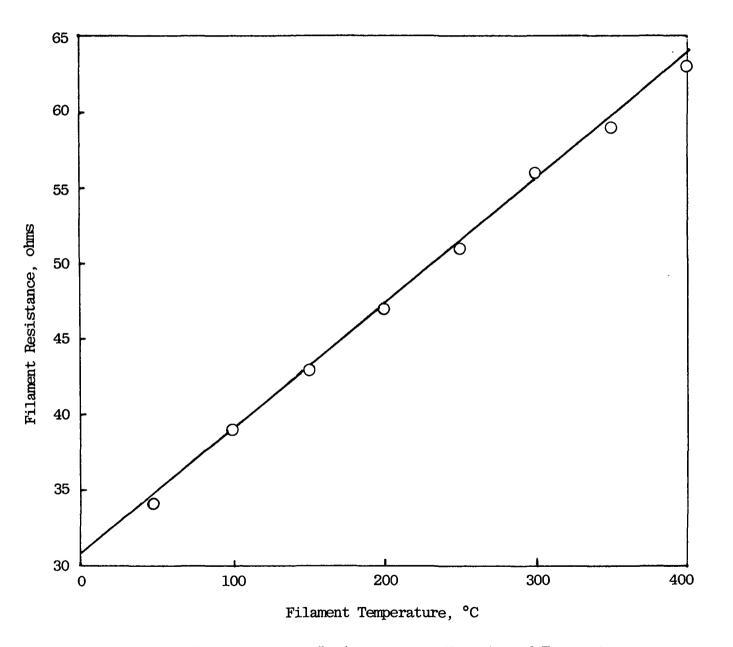


Figure IB-1. Filament Resistance as a Function of Temperature

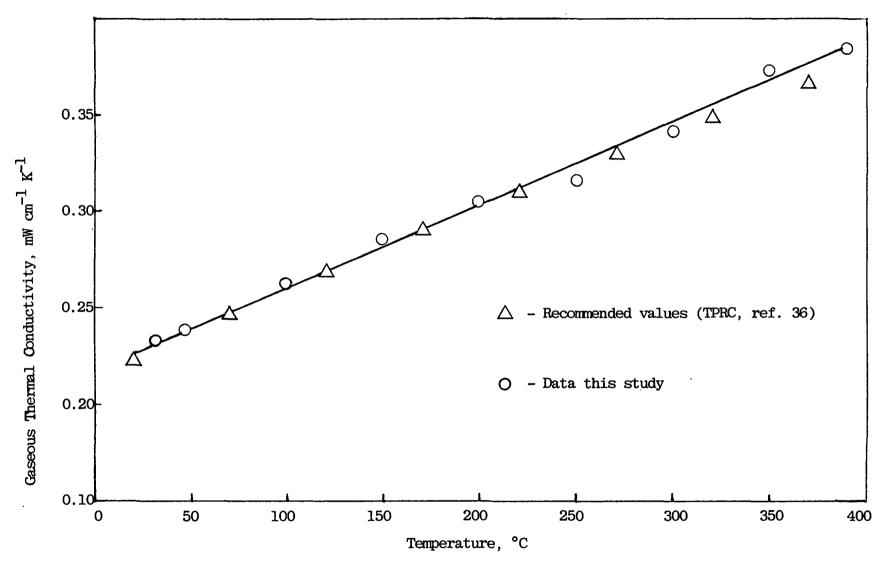


Figure IB-2 Apparatus Calibration with Argon

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### II. CHEMICAL ENGINEERING ANALYSES (TASK 2)

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#### A. Silane Process (Union Carbide)

Chemical engineering analysis activities were continued on the preliminary process design for the silane process (Union Carbide) during this reporting period.

Progress since the last reporting period for the process design is summarized given below for key guideline items:

	Prior	Current
Process Flow Diagram	75%	95%
Material Balance	50%	95%
Energy Balance	0%	50%
Property Data	40%	65%
Equipment Design	10%	60%

In current activities, primary efforts are being devoted to material balance, energy balance and equipment design for the revised flowsheet received from Mr. W.C. Breneman of Union Carbide.

#### B. CONVENTIONAL POLYSILICON PROCESS

Major resources and manpower were committed to the preliminary process design for the conventional polysilicon process. Initial review and modifications were completed, and results are presented. Design criteria were selected so that results would be comparable to alternate processes under consideration. Major modifications and key items are reviewed.

The detailed status sheet is shown in Table IIB-1.0 in order to present the items that make up the preliminary process design, and the preliminary process flowsheet is shown in Figure IIB-1.0.

The summarized results for the preliminary process design are presented in a tabular format to make it easier to locate items of specific interest. The guide for these tables is given below and represents the components that make up the complete design.

Base Case ConditionsTable	IIB-1.1
Reaction ChemistryTable	IIB-1.2
Raw Materials Requirements	IIB-1.3
Utility RequirementsTable	IIB-1.4
List of Major Process Equipment	IIB-1.5
Production Labor RequirementsTable	IIB-1.6

The tables should be self-explanatory, but a few comments are appropriate:

. The Base case conditions (Table IIB-1.1) were selected so that the designs and economic analyses prepared for alternate processes to produce solar cell grade silicon might be compared to the convential polysilicon process.

- . This poly plant is integrated to include
  - TCS production
  - TCS purification
  - Semiconductor grade silicon via rod reactors

. Proven commerical technology was assumed

- Fluidized bed reactor to produce TCS
- Distillation of TCS for purification
- Sieman's type rod (hair pin) reactor for product silicon
- References 20,31,32, and 33 for technical information
- . Raw Material Requirements (Table IIB-1.3)
  - HCl and M.G. Silicon are major items
- . Utility Requirements (Table IIB-1.4) - Electricity to operate rod reactors major item
- . Labor Requirements (Table IIB-1.6)
  - Most requirements estimated by method in reference 7.
  - For rod reactors, 1 operator per 10 reactors.

## TABLE IIB-1.0 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR CONVENTIONAL POLYSILICON PROCESS

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	Prel. Process Design Activity	Status		Prel. Process Design Activity	Status
1.	Specify Base Case Conditions 1. Plant Size 2. Product Specifics 3. Additional Conditions	• • •	7.	Equipment Design Calculations 1. Storage Vessels 2. Unit Operations Equipment 3. Process Data (P, T, rate, etc.) 4. Additional	•
2.	Define Reaction Chemistry 1. Réactants, Products 2. Equilibrium	• •	8.	List of Major Process Equipment 1. Size 2. Type	•
3.	Process Flow Diagram 1. Flow Sequence, Unit Operations 2. Process Conditions (T, P, etc.) 3. Environmental	•	8a.	3. Materials of Construction Major Technical Factors (Potential Problem Areas)	•
4.	<ul> <li>4. Company Interaction (Technology Exchange)</li> <li>Material Balance Calculations</li> <li>1. Raw Materials</li> </ul>	•	9.	<ol> <li>Materials Compatibility</li> <li>Process Conditions Limitations</li> <li>Additional</li> <li>Production Labor Requirements</li> </ol>	•
	<ol> <li>Products</li> <li>By-Products</li> </ol>	•		1. Process Technology 2. Production Volume	•
5.	Energy Balance Calculations 1. Heating 2. Cooling 3. Additional	• • •	10.	Forward for Economic Analysis	•
6.	Property Data 1. Physical 2. Thermodynamic 3. Additional	0 0 0		0 Plan • In Progress • Complete	

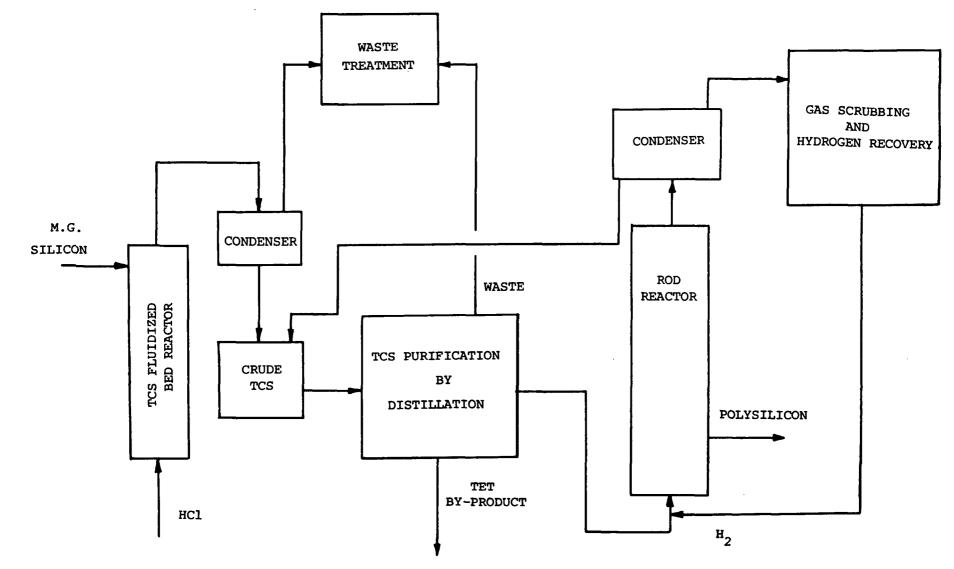


Figure IIB-1.0 Preliminary Process Flowsheet for Conventional Polysilicon Process

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BASE CASE CONDITIONS FOR CONVENTIONAL POLYSILICON PROCESS

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1.
     Plant Size
     ~ 1000 metric tons per year
     - Semiconductor grade silicon
2. Production of TCS
     - Fluidized Bed, 600<sup>°</sup>K, low pressure (65 PSIA)
     - Metallurgical grade silicon plus HCl gas
     - Chlorosilane content in condensed reator gas by moles (ref. 32)
          91.5% TCS (SiCl<sub>2</sub>H)
           5.2% TET (SiCl<sub>4</sub>)
           1.4% DCS (SiCl<sup>3</sup><sub>2</sub>H<sub>2</sub>)
            1.9% Heavies
     ~ Slight excess HCl in reator gas (1%)
     ~ Hydrogen burned
3. TCS Purification (ref. 31)
     - Distillation
     ~ 5% lights to waste (5% of TCS & TET)
     - Separate TCS and TET
     - 5% heavies from TCS & TET to waste
     - TET for by-product sales
     ~ TCS to rod reactor
4. Silicon Production
     - Rod reactor at 1050°C, 20 PSIA
     - Hydrogen to reduce TCS
     ~ Entering gas analysis
           10% TCS
          90% H<sub>2</sub>
     ~ 8.17 moles TCS in/mole of S; production in an operating reactor
     - Exit gas analysis (ref. 20)
          4.339% TET
          4.457% TCS
            .089% DCS
          2.197% HCl
         88.92% H
5. Waste Treatment
     - Light and heavy cuts from distillation to waste treatment
     - Vapors from TCS reactor condenser to scrubber
     - Vapor from rod reactor to scrubber
```

- All waste streams neutralized with NaOH

## TABLE IIB-1.1 (Continued)

- 6. Recycles
  - H<sub>2</sub> from rod reactor dried and returned, 5% losses
  - Chlorosilanes from rod reactor condensed off gas recycled to purification (distillation)
- 7. Operating Ratio
  - Approximately 90% utilization
  - Approximately 7880 hour/year production
- 8. Storage Considerations
  - Feed materials (two week supply)
  - Product (two week supply)
  - Process (several days)
- 9. Filament Pullers
  - Pull rate of 50-100 inches/hour
  - Average of 72 inches/hour used
  - 1/4" Filaments for silicon deposition needed

## REACTION CHEMISTRY FOR CONVENTIONAL POLYSILICON PROCESS

## 1. TCS Reactor

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si + 3 HCl → siHCl<sub>3</sub> + H<sub>2</sub> si + 4 HCl → siCl<sub>4</sub> + 2H<sub>2</sub> si + 2HCl → siH<sub>2</sub>Cl<sub>2</sub>

### 2. Rod Reactor

 $sihcl_{3} + H_{2} + si + 3hcl$   $sihcl_{3} + hcl + sicl_{4} + H_{2}$  $sihcl_{3} + H_{2} + sih_{2}cl_{2} + hcl$ 

3. Waste Treatment

 $\begin{aligned} \operatorname{SiHCl}_{3} + \operatorname{2H}_{2} \circ &\to \operatorname{SiO}_{2} + \operatorname{3HCl} + \operatorname{H}_{2} \\ \operatorname{SiCl}_{4} + \operatorname{2H}_{2} \circ &\to \operatorname{SiO}_{2} + \operatorname{4HCl} \\ \operatorname{SiH}_{2} \operatorname{Cl}_{2} + \operatorname{2H}_{2} \circ &\to \operatorname{SiO}_{2} + \operatorname{2HCl} + \operatorname{2H}_{2} \\ \operatorname{HCl} + \operatorname{NaOH} &\to \operatorname{NaCl} + \operatorname{H}_{2} \circ \end{aligned}$ 

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# RAW MATERIAL REQUIREMENTS FOR CONVENTIONAL POLYSILICON PROCESS

	Raw Material	Requirement lb/Kg of Silicon
1.	M.G. Silicon	6.72 Кg/Кg
2.	Anhydrous HCl	57.96
3.	Hydrogen	.828
4.	Caustic (50% NaOH)	53.29
5.	SiCl <sub>4</sub> (By Product)	46.12

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# UTILITY REQUIREMENTS FOR CONVENTIONAL POLYSILICON PROCESS

	UTILITY/FUNCTION		REQUIREMENTS/Kg OF SILICON PRODUCT
1.	Electricity		384.62 Kw-Hr
	1. All pump motors (16 motors)	(.339)	
	2. 2 compressor motors	(9.243)	
	3. Polysilicon Rod Reactor	(375)	
	4. Filament Pullers	(.0244)	
2.			152 Pounds
	1. HCl Vaporizer	(7.07)	
	2. Caustic Storage Tank	(1.82)	
	3. #1 Scrubber Vapor Heater	(.276)	
	4. #1 Distillation Column Calandria		
	5. #2 Distillation Column Calandria	• •	
	6. #3 Distillation Column Calandria		
	7. TCS Vaporizer	(10.79)	
	8. #2 Scrubber Vapor Heater	(3.4)	
	9. Liquid Recycle Heater	(5.52)	
	10. #4 Distillation Column Calandria		
	11. Rod Reactor	(-1287	
	II. ROU REACTOR	generate	a)
		generace	u)
3.	Cooling Water		
	1. TCS Reactor Off Gas Cooler	(13.91)	984.5 Gallons
	2. Rod Reactor Off Gas Cooler	(334)	
	3. #4 Distillation Column Condenser		
	4. Polysilicon Rod Reactor Cooling		
	End Plates	(473)	
	5. TCS Reactor Off Gas Compressor	(11.12)	
	6. Rod Reactor Off Gas Compressor	(115.2)	
		(,	
4.	Process Water		320.9 Gallons
	1. #2 Gas Scrubber	(31.36)	
	2. #1 Gas Scrubber	(134.82)	
	3. To Make Steam In Cooling Rod		
	Reactor Side Walls	(154.7)	
5.	Refrigerant (-40 <sup>0</sup> F)		42.1 M BTU
	1. TCS Reactor Off Gas Condenser	(12.57)	
	2. Rod Reactor Off Gas Condenser	(29.52)	
	0		
6.			92.3 M BTU
	1. #1 Distillation Column Condenser	(34)	
	2. #2 Distillation Column Condenser	(37.4)	
	3. #3 Distillation Column Condenser	(20.85)	
_			
7.			582 Pounds
	1. TCS Fluidized Bed Reactor	(581)	
	2. Nitrogen Heater	(0.61)	
-			
8.	Nitrogen	10	349.1 SCF
	1. Molecular Sieves	(328.5)	
	2. Polysilicon Rod Reactor Purge	(20.64)	

# LIST OF MAJOR PROCESS EQUIPMENT FOR CONVENTIONAL POLYSILICON PROCESS

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			The set of	Thursday	<b>D</b>	Size	Materials of Construction
			Туре	Function	Duty	5126	or construction
	1.	(Tl)	M.G. Silicon Storage Hopper	Raw Material Storage	2 Weeks Storage	$6.5 \times 10^4$ gallons	CS
	2.	(T2)	Liquid HCl Storage Tank	Raw Material Storage	2 Weeks Storage	2.5 x 10 <sup>5</sup> gallons 250 PSIA	Nickel Steel
	3.	(T3)	Crude TCS Hold Tanks (3)	Feed for Purification	l Week Storage	2.77 x 10 <sup>5</sup> gallons (each)	CS
	4.	(T4)	Waste Hold Tank	Feed For Waste Treatment	l Week Storage	$3.025 \times 10^4$ gallons	CS
	5.	(T5)	TCS Reactor Off Gas Flash Tank	Phase Separation		l ft. in diameter by 4 ft. tall, 300 PSIA	SS
23	6.	(T6)	Hydrogen Storage Tank	Make-up For Losses	8 Hours Backup for Pipeline Failure	7.24 x 10 <sup>4</sup> gallons Spherical 250 PSIA	CS
	7.	(T7)	Polysilicon Storage Space	Final Product Storage	2 Weeks Storage	1300 ft. <sup>3</sup> of space	CS
	8.	(T8)	TET Storage Tanks (2)	Final By-product Storage	2 Weeks Storage	l.62 x 10 <sup>5</sup> Gallons (each)	CS
	9.	(T9)	TET Feed Tanks (2)	Feed for Distillation Column #4	l Week Storage	8.83 x 10 <sup>4</sup> Gallons (each)	CS
	10.	(T10)	TCS Feed Tanks (3)	Feed for Distillation Column #3	l Day Storage	2.47 x 10 <sup>4</sup> Gallons (each)	CS
	11.	(Tll)	TCS Storage Tanks (3)	Purified TCS Hold-Up Feed to Rod Reactor	l Week Storage	l.64 x 10 <sup>5</sup> Gallons (each)	CS
	12.	(T12)	TET/TCS Feed Tanks (3)	Feed for Distillation Column #2	l Day Storage	3.75 x 10 <sup>4</sup> Gallons (each)	CS

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	13.	(T13)	Caustic Storage Tank	Raw Material Storage	2 Week Storage 1.91 x 10 <sup>5</sup> BTU/HR	1.82 x 10 <sup>5</sup> Gallons	SS
	14.	(T14)	#l Distillation Condenser Flash Tank	Phase Separation		l Ft. in Diameter by 4 Feet Tall	CS
	15.	(T15)	Rod Reactor Off Gas Flash Tank	Phase Separation		l Ft. in Diameter by 4 Feet Tall 300 PSIA	SS
	16.	(H1)	HCl Vaporizer	Vaporize Feed To TCS Reactor	7.5 x 10 <sup>5</sup> BTU/Hr	38.29 Ft. <sup>2</sup> 250 PSIA Shell	SS/SS
	17.	(H2)	TCS Reactor Off Gas Cooler	Cool Reaction Gas	4.4 x 10 <sup>5</sup> BTU/Hr	224 Ft. <sup>2</sup> 65 PSIA Tubes	CS/SS
24	18.	(H3)	TCS Reactor Off Gas Condenser	Condense Reaction Gas	1.6 x 10 <sup>6</sup> BTU/Hr	1423 Ft. <sup>2</sup> 300 PSIA Tubes	SS/SS
	19.	(H4)	#l Scrubber Vapor Heater	Heat Vapor Wastes to 40 <sup>0</sup> F for Scrubbing	3 x 10 <sup>4</sup> BTU/Hr	15.7 Ft. <sup>2</sup> 250 PSIA Shell	CS/SS
	20.	(Н5)	#1 Distillation Column Condenser	Condense Overheads for Relux	4.31 x 10 <sup>6</sup> BTU/Hr	1540 Ft. <sup>2</sup>	CS/SS
	21.	(Нб)	#l Distillation Column Calandria	Reboiler for Column #1	4 x 10 <sup>6</sup> BTU/Hr	311. Ft. <sup>2</sup> 250 PSIA Shell	CS/SS
	22.	(H7)	#2 Distillation Column Condenser	Condense Overheads For Reflux	4.7 x 10 <sup>6</sup> BTU/Hr	1555 Ft. <sup>2</sup>	CS/CS
	23.	(H8)	#2 Distillation Column Calandria	Reboiler for Column #2	5 x 10 <sup>6</sup> BTU/Hr	402.4 Ft. <sup>2</sup> 250 PSIA Shell	CS/SS
	24.	(H9)	#3 Distillation Column Condenser	Condense Overheads for Reflux	2.64 x 10 <sup>6</sup> BTU/Hr	867 Ft. <sup>2</sup>	CS/CS

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	25.	(H10)	#3 Distillation Column Calandria	Reboiler for Column #3	2.64 x 10 <sup>6</sup> BTU/Hr	173 Ft. <sup>2</sup> 250 PSIA Shell	CS/SS
	26.	(H11)	TCS Vaporizer	Vaporize Feed To Rod Reactor	1.13 x 10 <sup>6</sup> BTU/Hr	73 Ft. $^2$ 250 PSIA Shell	CS/CS
	27.	(H12)	Rod Reactor Off Gas Cooler	Cool Reaction Gas	1.06 x 10 <sup>7</sup> BTU/Hr	2519 Ft. <sup>2</sup> 20 PSIA	CS/SS
	28.	(H13)	Rod Reactor Off Gas Condenser	Condense Reaction Gas	3.74 x 10 <sup>6</sup> BTU/Hr	3341 Ft. <sup>2</sup> 300 PSIA Tubes	SS/SS
	29.	<u>(</u> H14)	#2 Scrubber Vapor Heater	Heat Vapor Wastes to 40 <sup>0</sup> F for Scrubbing	3.56 x 10 <sup>5</sup> BTU/Hr	180 Ft. <sup>2</sup> 250 PSIA Shell	CS/SS
	30.	(H15)	Liquid Recycle Heater	Heat Cold Recycle Liquid (Crude TCS) to 80 <sup>0</sup> F for Storage	5.79 x 10 <sup>5</sup> BTU/Hr	30.6 Ft. <sup>2</sup> 250 PSIA Shell	SS/SS
25	31.	(H16)	#4 Distillation Column Condenser	Condenser Overheads for Reflux	1.18 x 10 <sup>6</sup> BTU/Hr	513 Ft. <sup>2</sup>	cs/cs
	32.	(H17)	#4 Distillation Column Calandria	Reboiler for Column #4	1.18 x 10 <sup>6</sup> BTU/Hr	95 Ft. <sup>2</sup> 250 PSIA Shell	cs/ss
	33.	(H18)	Nitrogen Heater	Heat Regenerator Gas for Molecular Sieves	2.46 x 10 <sup>4</sup> BTU/Hr	44.8 Ft. <sup>2</sup>	cs/cs
	34.	(Pl)	TCS Reactor Off Gas Compressor	Compress Reaction Gas For Condensation	3.52 x 10 <sup>5</sup> BTU/Hr	138.2 Horsepower	CS
	35.	(P2)	Caustic Supply Pump	Supply Caustic for Waste Neutralization and Gas Scrubbers		9 gpm 100 Ft. of Head	SS
	36.	(P3)	#l Distillation Column Overheads Pump	Supply Reflux and Remove Waste to Waste Hold Tank		62.2 gpm 100 Ft. of Head	CS*

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	37.	(P4)	#l Distillation Column Calandria Pump	Forced Convection Pump		93 gpm 150 Ft. of Head	CS*
	38.	(P5)	TET/TCS Feed Pump	Feed #2 Distillation Column		26.1 gpm 100 Ft. of Head	CS*
	39.	(P6)	#2 Distillation Column Overheads Pump	Supply Relux, Pump Overhead to TCS Feed Tank		70 gpm 100 Ft. of Head	CS*
	40.	(P7)	TCS Feed Pump	Feed #3 Distillation Column		21 gpm 100 Ft. of Head	CS*
	41.	(P8)	#2 Distillation Column Calandria Pump	Forced Convection Pump		104 gpm 150 Ft. of Head	CS*
26	42.	(P9)	#3 Distillation Column Overhead Pump	Supply Reflux,Pump Overheads to TCS Storage Tank		39 gpm 100 Ft. of Head	CS*
	43.	(P10)	Rod Reactor TCS Feed Pump	Feed TCS to Rod Reactor		15 gpm 100 Ft. of Head	CS*
	44.	(P11)	#3 Distillation Column Calandria Pump	Forced Convection Pump		39 gpm 150 Ft. of Head	CS*
	45.	(P12)	Rod Reactor Off Gas Compressor	Compress Reaction Gas for Condensation	3.65 x 10 <sup>6</sup> BTU/Hr	1434 Horsepower	CS
	46.	(P13)	#4 Distillation Column Overheads Pump	Supply Reflux Pump TET by product to TET Storage Tank	<b>`</b>	21.59 gpm 100 Ft. of Head	CS*
	47.	(P14)	#4 Distillation Column Calandria Pump	Forced Convection Pump		22.4 gpm 100 Ft. of Head	CS*

NOTES

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\*Includes incremental higher cost for special purity requirements.

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	48.	(P15)	TET Feed Pump	Feed #4 Distillation Column		9.2 gpm 100 Ft. of Head	CS*
	49.	(P16)	Waste Treatment Pump	Pump from Waste Hold To Waste Treatment		2.8 gpm 50 Ft. of Head	CS
	50.	(P17)	Crude TCS Feed Pump	Feed Purification Area		28 gpm 100 Ft. of Head	CS*
	51.	(P18)	Process Water Feed Pump	Feed Process Water to Scrubber and Waste Treatment		350 gpm 100 Ft. of Head	CS
	52.	(C1)	#l Gas Scrubber	Scrub Gas Wastes from TCS Reactor Off Gas		43 Ft. Tall D = $3\frac{1}{2}$ Ft.	SS
	53.	(C2)	#2 Gas Scrubber	Scrub Gas Wastes from Hl6, H3, H5		40 Ft. Tall D = $2\frac{1}{4}$ Ft.	SS
27	54.	(C3)	#1 Distillation Column	Separate Light Impurities to Waste		29 Trays 24 inches äpart 3 3/4 Ft. in Diameter	CS
	55.	(C4)	#2 Distillation Column	Separate TET and TCS		29 Trays 24 inches apart 44 Ft. in Diameter	CS
	56.	(C5)	#3 Distillation Column	Separate Heavies TCS to Waste		15 Trays 20 inches apart 3 Ft. in diameter	CS
	57.	(C6)	#4 Distillation Column	Separate Heavies TET to Waste		15 Trays 20 inches apart 2¼ Feet in Diameter	CS
	58.	(Rl)	TCS Fluidized Bed Reactor	Production of TCS For Rod Reactor	4.552 x 10 <sup>6</sup> BTU/Hr (Cooling)	D = 2.61 Ft. L = 28.8 Ft. 64, 1" O D Cooling Tubes 9.4' Long	SS

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59. (R2)	Polysilicon Rod Reactors (305)	Production of Polysilicon		Hairpin Reactor (2 hair- pins, 3 Ft. long, 6 Inch Dia.)	Quartz
60. (Al)	Molecular Sieves (2)	Dry Out Rod Reactor Off Gas For Hydrogen Recycle		D = 3.5 Ft. L = 14.4 Ft.	CS
61. (A2)	Fines Separator	Remove Solids From Fluidized Bed Reactor Off Gas		12" Cyclone Separator	SS
62. (A3)	Hydrogen Flare	Dispose of Hydrogen Produced in TCS Fluidized Bed Reactor	8.94 x 10 <sup>6</sup> BTU/Hr	30 Feet High Stack 6" diameter	CS
63. (A4)	Filament Pullers	Production of 1/4" filamer Polysilicon depositon	nts for		

# PRODUCTION LABOR REQUIREMENTS FOR CONVENTIONAL POLYSILICON PROCESS

			Skilled La	abor	Semiskilled Labor		
	Unit Operation	Туре	Man Hrs/Day	Per Kg Si	Per Day	Per Kg Si	
1.	TCS Production	A	80	.0292			
2.	Vaporization	в	60	.0219			
3.	Vapor Compression	в	60	.0219			
4.	Vapor Condensation	в	60	.0219			
5.	TCS/TET Separation	С	40	.0146			
6.	TCS Purification	С	35	.0128			
7.	TET Purification	с	30	.011			
8.	Filament Pullers		120	.0438			
9.	Gas Scrubbing	A	64	.0232			
10.	Hydrogen Drying (Molecular Sieves)	В	32	.0117			
11.	Crude TCS Recycle System	В	58	.0212			
12.	Silicon Fines Sep- aration	В	15	.0055			
13.	Material Handling	А			90	.0329	
14.	Polysilicon Production		732	.2672	_		
	TOTAL		1386	.5059	90	.0329	

NOTES:

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- 1. A Batch Process or Multiple Small Units
  - **B** Average Process
  - C Automated Process
- 2. Man hours/day Unit from Figure 4-6, Peters and Timmerhaus (7).
- 3. Polysilicon manpower requirements based on batch operation with approximately 1 operator per 10 reactors.
- 4. Filament puller manpower requirements based on 1 operator per puller.

#### III. ECONOMIC ANALYSES (TASK 3)

3

A. Silane Process (Union Carbide)

Preliminary economic analysis activities were initiated during this reporting period for the silane process (Union Carbide).

Current activities are being devoted to cost estimation for mass transfer equipment required in the various separations and recycles in the process. The mass transfer equipment includes distillation towers, condensers, reboilers and accumulators.

#### B. Conventional Polysilicon Process

Economic analysis activities for the conventional polysilicon process were continued including preliminary review of raw materials, utilities, equipment and labor costs.

Primary efforts were devoted to the preliminary estimates of capital investment and product cost for the conventional polysilicon process. The status, including activities accomplished, in progress, and planned is shown in Table IIIB-1.

The initial results for the preliminary economic analysis are summarized in a tabular format. The guide for the tabular format is given below for the accompanying tables:

1.	Process Design InputsTable	IIIB-1.1
2.	Base Case ConditionsTable	IIIB-1.2
3.	Raw Material CostTable	IIIB-1.3
4.	Utility CostTable	IIIB-1.4
5.	Major Process Equipment CostTable	IIIB-1.5
6.	Production Labor CostTable	IIIB-1.6

The process design inputs are given in Table IIIB-1.1 including raw materials, utilities, equipment and labor requirements. The base case conditions for the preliminary cost analysis are presented in Table IIIB-1.2 including the reference 1975 time period.

The preliminary estimate of cost for raw materials, utilities, major process equipment and labor required for the production of silicon in the conventional polysilicon process are detailed in Table IIIB-1.3 to IIIB-1.6.

In Table IIIB-1.4 for utilities, a value of 3¢/kw-hr represents a high electrical cost. On the other end of the range, a value of 1.5¢/kw-hr represents a low electrical cost. A value of 2.25¢/kw-hr would represent an intermediate electrical cost.

Electrical costs vary with location (different costs for different states and different costs for different regions in the same state). However, the range (1.5-3¢/kw-hr) and intermediate value (2.25¢/kw-hr) are considered representative based on a recent plant site survey (ref. 35) listing industrial power cost in the USA. With respect to the intermediate value, the survey indicated the following average statewide cost for industrial power: Michigan (2.48), Arizona (2.27), Missouri (2.05) and Texas (1.49).

Upon completion of the preliminary review in the areas of major process equipment, utilities and production labor costs, major activities focused on estimates of plant investment and product costs for the production of semiconductor grade polysilicon via the conventional hairpin process technology. Three cases were considered (Case A, B and C). Each case is discussed separately.

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# ECONOMIC ANALYSES: PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR CONVENTIONAL POLYSILICON PROCESS

Status	•	•	•	•		•	•	۲	•	•	•			•	•	•	9	3	9	đ					
Prel. Process Economic Activity	Production Labor Costs	1. Base Cost Per Man Hour	<ol><li>Cost/Kg Silicon Per Area</li></ol>	3. Total Cost/Kg Silicon		Estimation of Plant Investment	1. Battery Limits Direct Costs	2. Other Direct Costs	3. Indirect Costs	4. Contingency	5. Total Plant Investment	(Fixed Capital)	ŕ	Estimation of Total Product Cost	1. Direct Manufacturing Cost	2. Indirect Manufacturing Cost	3. Plant Overhead	4. By-Product Credit	5. General Expenses	6. Total Cost of Product				ln Progress	
	6.					7.								æ.											
Status	•	•	0	•	•		•	•	•	9		•	•	•	0		۲	•	S	•	•	•	•		
Prel. Process Economic Activity	Process Design Inputs	l. Raw Material Requirements	2. Utility Requirements	3. Equipment List	4. Labor Requirements		Specify Base Case Conditions	l. Base Year for Costs	2. Appropriate Indices for Costs	3. Additional		Raw Material Costs	<ol> <li>Base Cost/Ib. of Material</li> </ol>	<ol><li>Material Cost/Kg of Silicon</li></ol>	3. Total Cost/Kg of Silicon		Utility Costs	1. Base Cost for Each Utility	2. Utility Cost/Kg of Silicon	3. Total Cost/Kg of Silicon	Major Process Equipment Costs	l. Individual Equipment Cost	2. Cost Index Adjustment		
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## PROCESS DESIGN INPUTS FOR CONVENTIONAL POLYSILICON PROCESS

- 1. Raw Material Requirements
   -M.G. silicon, anhydrous HCl, caustic, hydrogen, silicon tetrachloride (by-product)
   -see table for "Raw Material Cost"
- 2. Utility
   -electrical, steam, cooling water, etc.
   -see table for "Utility Cost"

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- 3. Equipment List -63 pieces of major process equipment -process vessels, heat exchangers, reactor, etc. -see table for "Major Process Equipment Cost"
- 4. Labor Requirements -production labor for deposition, vaporization, product handling, etc. -see table for "Production Labor Cost"

## BASE CASE CONDITIONS FOR CONVENTIONAL POLYSILICON PROCESS

- 1. Capital Equipment
  -January 1975 Cost Index for Capital Equipment Cost
  -January 1975 Cost Index Value = 430
- 2. Utilities -Electrical, Steam, Cooling Water, Nitrogen -January 1975 Cost Index (U.S. Dept. Labor) -Values determined by literature search and summarized in cost standardization work
- Raw Material Cost

   Chemical Marketing Reporter
   January 1975 Value
   Other Sources

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4. Labor Cost -Average for Chemical Petroleum, Coal and Allied Industries (1975) -Skilled \$6.90/hr -Semiskilled \$4.90/hr

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# RAW MATERIAL COST FOR CONVENTIONAL POLYSILICON PROCESS

Ra	w Material	Requirement lb/Kg of Silicon	\$/lb of Material	Cost \$/Kg Of Silicon
1.	M.G. Silicon	6.72 (Kg/Kg)	1.0/Kg (Ref.33)	6.72
2.	Anhydrous HCl	57.96	.10 (Ref. 34)	5.79
3.	Hydrogen	.828	.96 (Ref. 33)	.79
4.	Caustic (50% NaOH	() 53.29	.0382 (Ref. 12)	2.04
5.	$siCl_4$ (By Product	.) 46.12	.135 (Ref. 12)	6.23 (credit)

TOTAL COST \$ 9.11/Kg Silicon

# UTILITY COST FOR CONVENTIONAL POLYSILICON PROCESS

	Utility	Requirements/Kg of Silicon	Cost of Utility	Cost \$/Kg of Silicon
1.	Electricity	384.6 Kw-hr	\$ .03/kw-hr	\$ 11.54
2.	Steam	152 Pounds	~ *	-
3.	Cooling Water	984.5 Gallons	\$ .08/M Gal.	.08
<i>,</i> 4.	Process Water	320.9 Gallons	\$ .35/M Gal.	.11
5.	Refrigerant (-40 <sup>0</sup> F)	42.1 M BTU	\$10.38/MM BTU	.44
6.	Refrigerant (34 <sup>0</sup> F)	92.3 M BTU	\$ 3.75/MM BTU	.35
7.	High Temperature Coolant	, 582 Pounds	\$ 2.7/M Pounds	1.57
8.	Nitrogen	349 SCF	\$ .50/M SCF	.17
			TOTAL COST	\$14.26/Kg Silicon

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\* All steam produced by cooling jacket on polysilicon rod reactor.

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# PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR CONVENTIONAL POLYSILICON PROCESS

	Equip	nent	Purchased Cost, \$M
1.	(Tl)	M.G. Silicon Storage Hopper	24.1
2.	(T2)	Liquid HCl Storage Tank	435.96
3.	(T3)	Crude TCS Hold Tank (3)	178.8
4.	(T4)	Waste Hold Tank	14.9
5.	(T5)	TCS Reactor Off Gas Flash Tank	7.2
6.	(T6)	Hydrogen Storage Tank	152.1
7.	(т7)	Polysilicon Storage Space	10.8
8.	(T8)	Tet Storage Tanks (2)	85.2
9.	(T9)	Tet Feed Tanks (2)	57.8
10.	(T10)	TCS Feed Tanks (3)	42.6
11.	(Tll)	TCS Storage Tanks (3)	127.8
12.	(T12)	TET/TCS Feed Tanks (3)	54.
13.	(T13)	Caustic Storage Tank	106.7
14.	(Tl4)	#1 Distillation Condenser Flash Tank	.85
15.	(T15)	Rod Reactor Off Gas Flash Tank	7.2
16.	(Hl)	HCl Vaporizer	2.5
17.	(H2)	TCS Reactor Off Gas Cooler	7
18.	(H3)	TCS Reactor Off Gas Condenser	46.3
19.	(H4)	#1 Scrubber Vapor Heater	.75
20.	(H5)	#1 Distillation Column Condenser	14.
21.	(H6)	#1 Distillation Column Calandria	9.25
22.	(H7)	#2 Distillation Column Condenser	14.6
23.	(H8)	#2 Distillation Column Calandria	11.92
24.	<b>(</b> H9)	#3 Distillation Column Condenser	9.1
25.	(H10)	#3 Distillation Column Calandria	5.8
26.	(H11)	TCS Vaporizer	1.8
27.	(H12)	Rod Reactor Off Gas Cooler	49.4
28.	(H13)	Rod Reactor Off Gas Condenser	97.5
29.	(H14)	#2 Scrubber Vapor Heater	5.8
30.	(H15)	Liquid Recycle Heater	2.3
31.	(H16)	#4 Distillation Column Condenser	6.4
32.	(H17)	#4 Distillation Column Calandria	3.7
33.	(H18)	Nitrogen Heater	1.3

# TABLE IIIB-1.5 (Continued)

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34.	(Pl)	TCS Reactor Off Gas Compressor	53.2
35.	(P2)	Caustic Supply Pump	1.56
36.	(P3)	#1 Distillation Column Overheads Pump	2.64
37.	(P4)	#1 Distillation Column Calandria Pump	3.83
38.	(P5)	TET/TCS Feed Pump	2.04
39.	(P6)	#2 Distillation Column Overhead Pump	2.8
40.	(P7)	TCS Feed Pump	1.8
41.	(P8)	#2 Distillation Column Calandria Pump	3.8
42.	(P9)	#3 Distillation Column Overhead Pump	2.2
43.	(P10)	Rod Reactor TCS Feed Pump	1.7
44.	(P11)	#3 Distillation Column Calandria Pump	2.6
45.	(P12)	Rod Reactor Off Gas Compressor	235.5
46.	(P13)	#4 Distillation Column Overheads Pump	1.87
47.	(P14)	#4 Distillation Column Calandria Pump	1.87
48.	(P15)	TET Feed Pump	1.56
49.	(P16)	Waste Treatment Pump	.77
50.	(P17)	Crude TCS Feed Pump	1.9
51.	(P18)	Process Water Feed Pump	3.7
52.	(Cl)	#1 Gas Scrubber	53.2
53.	(C2)	#2 Gas Scrubber	29.
54.	(C3)	#1 Distillation Column	26.1
55.	(C4)	#2 Distillation Column	27.7
56.	(C5)	#3 Distillation Column	8.9
57.	(C6)	#4 Distillation Column	6.7
58.	(R1)	TCS Fluidized Bed Reactor	57.2
59.	(R2)	Polysilicon Rod Reactors (305)	56. (each)
60.	(Al)	Molecular Sieves	16.77
61.	(A2)	Fines Separator	4.8
62.	(A3)	Hydrogen Flare	1.
63.	(A4)	Filament Pullers (5)	<u>    15. (</u> each)
		TOTAL PURCHASED COST	\$19,307.14

# PRODUCTION LABOR COST FOR CONVENTIONAL POLYSILICON PROCESS

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	Unit Operation	Skilled Labor Man-Hrs/Kg Si	Semiskilled Labor Man-Hrs/Kg Si	Cost \$/Kg Si
1.	TCS Production	.0292		.2014
2.	Vaporization	.0219		.1511
3.	Vapor Compression	.0219		.1511
4.	Vapor Condensation	.0219		.1511
5.	TCS/TET Separation	.0146		.1007
6.	TCS Purification	.0128		.0883
7.	TET Purification	.011		.0759
8.	Filament Pullers	.0438		.3021
9.	Gas Scrubbing	.0232		.1600
10.	Hydrogen Drying (Molecular Sieves)	.0117		.0807
11.	Crude TCS Recycle System	.0212		.1463
12.	Silicon Fines Separation	.0055		.038
13.	Materials Handling		.0329	.1612
14.	Polysilicon Production	.2672		1.8429
			TOTAL COST	\$3.65/Kg Silicon

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Based on labor costs of \$6.90 skilled, \$4.90 semiskilled.

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# ESTIMATION OF PLANT INVESTMENT COST FOR CONVENTIONAL POLYSILICON PROCESS

	İnvestment	: (\$1000)
	1975 Plant	1960's Plant
1. DIRECT PLANT INVESTMENT COSTS		· <u></u>
1. Major Process Equipment Cost	19,307	11,032
2. Installation of Major Process Equipment	4,699	2,685
3. Process Piping, Installed	8,969	5,125
4. Instrumentation, Installed	924	528
5. Electrical, Installed	1,931	1,103
·	3,303	-
6. Process Buildings, Installed	3,303	1,889
la. SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	39,133	22,362
2. OTHER DIRECT PLANT INVESTMENT COSTS		
1. Utilities, Installed	9,096	5,198
2. General Services, Site Development,		•
Fire Protection, etc.	2,317	1,324
3. General Buildings, Offices, Shops, etc.	5,104	2,917
4. Receiving, Shipping Facilities	4,741	2,709
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2a. SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS		
(PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIM	17S) 21,258	12,147
	110,	
3. TOTAL DIRECT PLANT INVESTMENT COST, la + 2a	60,391	34,509
4. INDIRECT PLANT INVESTMENT COSTS		
1. Engineering, Overhead, etc.	3,757	2,147
2. Normal Cont. for Floods, Strikes, etc.	9,076	5,186
2. Normal cont. for floods, scilles, etc.	57010	5,100
4a. TOTAL INDIRECT PLANT INVESTMENT COST	12,833	7,333
5. TOTAL DIRECT AND INDIRECT PLANT INVESTMENT	73,224	41,842
COST, 3 + 4a		
6. OVERALL CONTINGENCY, % OF 5 @10%	7,322	4,184
		46.006
7. FIXED CAPITAL INVESTMENT FOR PLANT, $5 + 6$	80,546	46,026
8. WORKING CAPITAL INVESTMENT FOR PLANT, % OF 7 @ 158	12,082	6,904
9. TOTAL PLANT INVESTMENT, 7 + 8	92,628	52,930
1975 CE Plant Cost Index = 182		
1965 CE Plant Cost Index = $102$	Plant	Plant
1960 CE Plant Cost Index = 104	Constructed	Constructed
1900 CE Flanc Cost Index ~ 102	In 1975	In 1960's (1965 or Earlier)

#### 1. Case A

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Case A is based on 1975 costs for plant constructed in 1975. Range reflects low and high electrical costs (1.5-3.0¢/KW.HR). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

Plant investment and product cost estimates are summarized below:

- . Process..... Process
- . Plant Size.....Year
- . Plant Product......Semiconductor Grade Polysilicon
- . Plant Investment......\$92,600,000
- . Product Cost (Sales Price).....63.6-70.3\$/KG Si @ 10% ROI

The product cost of 63.6-70.3\$/KG Si includes a 10% ROI (return on investment).

The product cost (sales price) at different levels of return on investment (ROI) is given in Table IIIB-1.8A. More detailed data for plant investment and product cost are presented in the Appendix (A.1 and A.2).

#### TABLE IIIB - 1.8A

PRODUCT COST (SALES PRICE) VS. RETURN ON INVESTMENT (ROI): CASE A

- . Process..... Process
- . Plant Size..... 1,000 Metric Tons/Year

. Plant Product..... Semiconductor Grade Polysilicon

. Plant Investment..... \$92,600,000

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. Product Cost With Profit (Sales Price)	Range,\$/KG	Intermed. \$/KG
0% ROI	45.1-51.8	48.4
10% ROI	63.6-70.3	67.0
20% ROI	82.2-88.8	85.5
25% ROI	91.4-98.1	94.7
30% ROI	101-107	104
40% ROI	119-126	123

Basis: Case A is based on 1975 costs for plant constructed in 1975. Range reflects low and high electrical costs (1.5-3.0¢/KW.HR). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

#### 2. Case B

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Case B is based on 1975 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

The plant investment and product cost estimates are summarized below:

.Process	.Conventional Polysilicon Process
.Plant Size	.1,000 Metric Tons/Year
.Plant Product	.Semiconductor Grade Polysilicon
.Plant Investment	.\$52,900,000
.Product Cost (Sales Price)	.61.1-67.7\$/KG Si @ 25% ROI

The product cost of 61.1-67.7\$/KG Si includes a 25% ROI (return on investment).

The variation of product cost (sales price) with return on investment (ROI) is given in Table IIIB-1.8B. More detailed data for plant investment and product cost are presented in the Appendix (B.1 and B.2).

#### TABLE IIIB - 1.8B

PRODUCT COST (SALES PRICE) VS. RETURN ON INVESTMENT (ROI): CASE B

- . Process..... Conventional Polysilicon Process . Plant Size..... 1,000 Metric Tons/Year
- . Plant Product..... Semiconductor Grade Polysilicon
- . Plant Investment..... \$52,900,000

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. Product Cost With Profit (Sales Price)	Range,\$/KG	Intermed. \$/KG
0% ROI	34.7-41.3	38.0
10% ROI	45.2-51.9	48.6
20% ROI	55.8-62.5	59.1
25% ROI	61.1-67.7	64.4
30% ROI	66.3-73.0	69.7
40% ROI	76.9-83.6	80.3

Basis: Case B is based on 1975 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR), Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

#### 3. Case C

Case C is based on 1977 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR plus 20% escalation). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR plus 20% escalation). This case probably best represents the current situation for polysilicon production of semiconductor grade via the conventional hairpin process technology.

The plant investment and product cost estimates are summarized below:

- . Process..... Process..... Process
- . Plant Size.....Year
- . Plant Product......Semiconductor Grade Polysilicon
- . Plant Investment.....\$52,900,000

The product cost of 64.8-72.7\$/KG Si includes a 25% ROI (return on investment).

The product cost (sales price) at various levels of return on investment (ROI) is presented in Table IIIB-1.8C. More detailed data for plant investment and product cost are presented in the Appendix (C.1 and C.2).

#### TABLE IIIB - 1.8C

PRODUCT COST (SALES PRICE) VS. RETURN ON INVESTMENT (ROI): CASE C

- . Process..... Process

. Plant Product......Semiconductor Grade Polysilicon

. Plant Investment......\$52,900,000

. Product Cost With Profit (Sales Price)	Range,\$/KG	Intermed.,\$/KG
0% ROI	38.3-46.3	42.3
10% ROI	48.9-56.9	52.9
20% ROI	59.5-67.4	63.5
25% ROI	64.8-72.7	68.8
30% ROI	70.1-78.0	74.0
40% ROI	80.6-88.6	84.6

Basis: Case C is based on 1977 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR plus 20% escalation). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR plus 20% escalation).

#### IV. SUMMARY - CONCLUSIONS

The following summary-conclusions are made as a result of major activities accomplished in this reporting period:

1. Task 1

Major efforts were continued for process system properties of silicon source materials under consideration for solar cell grade silicon including data collection, analysis estimation and correlation.

The vapor pressure of silicon tetrachloride was correlated as a function of temperature using the following equation:

$$\log P_v = A + \frac{B}{T} + C \log T + DT + ET^2$$

Values for the correlation constants A, B, C, D and E are presented. The versatile correlation covers both low and high pressure regions with good agreement of calculated and experimental data. Average absolute deviation was only 0.7% for fifty-eight data points tested.

Heat capacity data for the gas phase were correlated by a series expansion in temperature:

$$C_{p} = A + BT + CT^{2} + DT^{3}$$

The correlation constants were determined from a least-squares fit of the available data from American, Russian, German and Japanese sources.

The calibration of the apparatus for measuring thermal conductivity of gases from 25°C to 400°C was completed. The accuracy of data to be obtained from this instrument was evaluated by making thermal conductivity measurements for argon between 25°C and 400°C. The thermal conductivity values obtained in this study were in excellent agreement with recommended values from the literature (ref.36). Deviations were only  $\pm 2$ % up to 300°C and  $\pm 4$ % up to 400°C.

## 2. Task 2

Chemical engineering analysis of the silane process (Union Carbide) was continued using the revised flowsheet from Mr. W.C. Breneman. Material balance is about 95% complete for the preliminary design. Energy balance, property data and equipment design are about 60% complete.

The review and modification of the conventional polysilicon process preliminary process design has been completed, and results are presented. Major items modified include the rod reactor area, waste treatment area, and labor requirements. Key items are HCl and M.G. Silicon consumption, electrical requirements for the rod reactors, and the rod reactor area.

3. Task 3

Economic analysis activities for the production of semiconductor grade polysilicon via the conventional hairpin process technology were continued including completion of the preliminary review in the areas of major process equipment, utilities and production labor costs.

Three cases for the conventional polysilicon process were considered (Case A, B and C). Results are summarized below with the range reflecting low and high electrical costs:

- 1. Case A
   . Product Cost (Sales Price)..........63.6-70.3\$/KG Si @ 10% ROI
- 2. Case B
   . Product Cost (Sales Price).....61.1-67.7\$/KG Si @ 25% ROI

Case C probably best represents the current situation for polysilicon production of semiconductor grade. It is based on current 1977 costs (raw materials, labor, utilities, etc.) for a poly plant constructed in the 1960's. Most poly plants in the U.S.A. were constructed in 1960's or earlier and are producing polysilicon at current operating costs (labor, utilities, etc.). The product cost (sales price) of 64.8-72.7\$/KG Si includes a profit of 25% ROI (return on investment). V. PLANS

Plans for the next reporting period are summarized below:

1. Task 1

Continue analyses of process system properties for silicon source materials under consideration for solar grade silicon.

Perform additional correlation activities on experimental data.

Further evaluation of the instrument will be made by measuring the thermal conductivity of hydrogen in the temperature range 25°C to 400°C. Thermal conductivity measurements will be initiated for silane and the chlorinated silanes.

2. Task 2

Design activity on the silane process will continue.

3. Task 3

Initiate cost analysis of the silane process (Union Carbide).

Perform additional economic analyses as information is received from design activities for processes under consideration for production of solar cell grade silicon.

#### References

1. Bauman, H. C., "Fundamentals of Cost Engineering In the Chemical Industry," Reinhold Publishing Corp., N.Y. (1964).

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- Chilton, C. H., ed., "Cost Engineering In the Process Industries," McGraw-Hill Book Co., N.Y. (1960).
- Evans, F. L., Jr., "Equipment Design Handbook for Refineries and Chemical Plants," Vol. I and II, Gulf Publishing, Houston (1971 and 1974).
- 4. Guthrie, K. M., "Process Plant Estimating Evaluation and Control," Craftsman Book Company of America, Solana Beach, Calif. (1974).
- 5. Happel, J., and Jordan, D. G., "Chemical Process Economics," 2nd edition, Marcel Dekker, Inc., N.Y. (1975).
- Perry, R. H., and Chilton, C. H., "Chemical Engineers' Handbook," 5th edition, McGraw-Hill Book Co., N.Y. (1973).
- Peters, M. S., and Timmerhaus, K. D., "Plant Design and Economics for Chemical Engineers," 2nd edition, McGraw-Hill Book Co., N.Y. (1968).
- Popper, H., ed., "Modern Cost-Engineering Techniques," McGraw-Hill Book Co., N.Y. (1970).
- 9. Winter, O., Ind. Eng. Chem., 61 (4), 45 (1969).
- Perry, R. H., and Chilton, C. H., "Chemical Engineers' Handbook," 5th edition, McGraw-Hill, N.Y. (1973).
- 11. Jelen, F. C., "Cost And Optimization Engineering," McGraw-Hill, N.Y. (1970).
- "Chemical Marketing Reporter," Schnell Publishing Company, New York (Jan. 1975).
- "Wholesale Prices and Prices Indexes," U.S. Dept. of Labor, U.S. Government Printing Office, Washington D.C. (March 1975).
- Anon. "Costs for Building and Operating Aluminum Producing Plants," Chem. Eng., 120 (Sept. 1963).
- 15. Zimmerman, O. T. and Lavine, I., "Cost Eng.," 6, 16, (July 1961).
- 16. "Monthly Labor Review,"U.S. Dept. of Labor, Bureau of Labor Statistics, (June 1976).

17. del Valle, Eduardo G., "Evaluation of the Energy Transfer in the Char Zone During Ablution," Louisiana State University Ph.D. Thesis, December 15, 1974.

- 18. Balzhiser, R. E., Samuels, M. R. and Eliassen, J. D., <u>Chemical Engineering</u> Thermodynamics, Prentice-Hall, Inc., 1972.
- 19. Hunt, C. P. and Sirtl, E., J. Electrochem Soc., <u>119</u> (No. 12) 1741 (December 1972).
- Bawa, M. S., Goodman, R. C., and J. K. Truitt, "Kinetics and Mechanism of Deposition of Silicon by Reduction of Chlorosilanes with Hydrogen," Chem. Vap. Dep. 4th Int. Conf. (1973).
- 21. Uhl, V.W. and Hawkins, A.W., "Technical Economics for Engineers", A.I.Ch.E. Continuing Education Series 5, A.I.Ch.E., New York (1976).
- 22. Woods, D. R., "Financial Decision Making in the Process Industry", Prentice Hall, Inc. (1975).
- 23. Ludwig, E. E., "Applied Project Management for the Process Industries", Gulf Publishing Co. (1974).
- 24. Guthrie, K.M., Chem. Eng., p.114 (March 24, 1969). Available as reprint "Capital Cost Estimating" from Chemical Engineering, N.Y.
- 25. Haselbarth, J.E., and J.M. Berk, Chem. Engr., p.158 (May 16, 1960).
- 26. Baasel, W.D., "Preliminary Chemical Engineering Plant Design", American Elsevier Publishing Company, Inc. (1976).
- 27. Garcia-Borras, T., Hydrocarbon Processing, 55 (12), 137 (Dec., 1976).
- 28. Holland, F.A., F.A. Watson, and J.K. Wilkinson, "Introduction to Process Economics", John Wiley & Sons, London (1974).
- 29. Winton, J.M., Chemical Week p.35 (Nov. 10, 1976).
- 30. Garcia-Borras, T., Hydrocarbon Processing, 56 (1), 171 (Jan. 1977).
- 31. Boggs, B.E., T.G. Digges, Jr., M.A. Drews, and C.L. Yaws, "High Purity Silicon Manufacturing Facility", Government Report AFML-TR-71-130, July 1971.
- 32. Breneman, W.C. and J.Y.P. Mui, Quarterly Progress Report, April 1976, JPL Contract 954334.

- 33. Blocher, J.M., Jr., M.F. Browning, W.J. Wilson, and D.C. Carmichael, Second Quarterly Progress Report (12/15/75) to 3/31/1976) April 8, 1976 of Battelle Columbus Laboratories.
- 34. Dr. Leon Crossman, Dow Chemical Company, Personal Communication, 1977.

•

- 35. Winton, J. M., "Plant Sites 1977", Chemical Week, <u>119</u>, No. 19, p. 35 (Nov. 10, 1976).
- 36. Touloukian, T.S. (Series Editor) and others, "Themphysical Properties Of Matter", Volumes 1-13, 1st and 2nd editions, IKI/Plenum Press, New York (1970-1976).

## APPENDIX A.1

## ESTIMATION OF PRODUCT COST FOR CONVENTIONAL POLYSILICON PROCESS: CASE A

PRODUCT COST, \$/KG Si

		LOW 1.5¢/KW.HR	HIGH 3¢/KW.HR	INTERMED. 2.25¢/KW.HR
1.	Direct Manufacturing Cost (Direct Cost)			
	1. Raw Materials	15.34	15.34	15.34
	2. Direct Operating Labor	3.65	3.65	3.65
	3. Utilities	8.49	14.26	11.37
	4. Supervision and Clerical	.55	.55	.55
	5. Maintenance and Repairs	2.16	2.16	2.16
	6. Operating Supplies	.43	.43	.43
	7. Laboratory Charge	.55	.55	· <b>.</b> 55
2.	Indirect Manufacturing Cost (Fixed Cost)			
	1. Depreciation	8.05	8.05	8.05
	2. Local Taxes	1.61	1.61	1.61
	3. Insurance	.81	.81	.81
3.	Plant Overhead	3.82	3.82	3.82
4.	By-Product Credit	(6.23)	(6.23)	(6.23)
4a.	Total Manufacturing Cost, $1 + 2 + 3 + 4$	39.23	45.00	42.11
5.	General Expenses			
	1. Administration	2.35	2.70	2.53
	2. Distribution and Sales	2.35	2.70	2.53
	3. Research and Development	1.18	1.35	1.26
6.	Product Cost Without Profit, 4a + 5	45.11	51.75	48.43
7.	Profit For Product (After Taxes)			

8. Product Cost With Profit, 6 + 7

.

Basis: Case A is based on 1975 costs for plant constructed in 1975. Range reflects low and high electrical costs (1.5-3.0¢/KW.HR). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

## APPENDIX A.2

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PRODUCT COST VARIATION (SALES PRICE) WITH RETURN ON INVESTMENT (ROI): CASE A

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PRODUCT COST WITH PROFIT: SALES PRICE, \$/KG Si

•	Process	Conventional	Polysilicon	Process
•	Plant Size	1,000 Metric	Tons/Year	
	Plant Product	Semiconducto	r Grade Polys	silicon
•	Plant Investment	\$92,600,000		

RETURN ON INVESTMENT AFTER TAXES %ROI	LOW 1.5¢/KW.HR	HIGH 3¢/KW.HR	INTERMED. 2.25¢/KW.HR
0	45.11	51.75	48.43
5%	54.37	61.01	57.69
10%	63.63	70.27	66.95
15%	72.89	79.53	76.21
20%	82.15	88.79	85.47
25%	91.41	98.05	94.73
30%	100.67	107.31	103.99
40%	119.19	125.83	122.51
50%	137.71	144.35	141.03
60%	156.23	162.87	159.55

## APPENDIX B.1

# ESTIMATION OF PRODUCT COST FOR CONVENTIONAL POLYSILICON PROCESS: CASE B

		PRODUCT COST, \$/KG Si								
		LOW 1.5¢/KW.HR	HIGH 3¢/KW.HB	INTERMED. 2.25¢/KW.HR						
1.	Direct Manufacturing Cost (Direct Cost)									
	1. Raw Materials	15.34	15.34	15.34						
	2. Direct Operating Labor	3.65	3.65	3.65						
	3. Utilities	8.49	14.26	11.37						
	4. Supervision and Clerical	.55	.55	.55						
	5. Maintenance and Repairs	2.16	2.16	2.16						
	6. Operating Supplies	.43	.43	.43						
	7. Laboratory Charge	.55	.55	.55						
2.	Indirect Manufacturing Cost (Fixed Cost)									
	1. Depreciation									
	2. Local Taxes	.92	.92	.92						
	3. Insurance	.46	.46	.46						
3.	Plant Overhead	3.82	3.82	3.82						
4.	By-Product Credit	(6.23)	(6.23)	(6.23)						
4a.	Total Manufacturing Cost, $1 + 2 + 3 + 4$	30.14	35.91	33.02						
5.	General Expenses									
	1. Administration	1.81	2.15	1.98						
	2. Distribution and Sales	1.81	2.15	1.98						
	3. Research and Development	.90	1.08	.99						
6.	Product Cost Without Profit, 4a + 5	34.66	41.29	37.97						
7.	Profit For Product (After Taxes)									

8. Product Cost With Profit, 6 + 7

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Basis: Case B is based on 1975 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR).

# APPENDIX B.2

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PRODUCT COST VARIATION (SALES PRICE) WITH RETURN ON INVESTMENT (ROI): CASE B

•	Process	Conventional	Polysili	con Process
	Plant Size			
•	Plant Product	Semiconducto	r Grade P	olysilicon
•	Plant Investment	\$52,900,000		

PRODUCT COST WITH PROFIT:

	SALE	S PRICE, \$/K	<u>G Si</u>				
RETURN ON INVESTMENT AFTER TAXES &ROI	LOW 1.5¢/KW.HR	HIGH 3¢/KW.HR	INTERMED. 2.25¢/KW.HR				
0	34.66	41.29	37.97				
5%	39.95	46.58	43.26				
10%	45.24	51.87	48.55				
15%	50.53	57.16	53.84				
20%	55.76	62.45	59.13				
25%	61.05	67.74	64.42				
30%	66.34	73/03	69.71				
40%	76.92	83.61	80.29				
50%	87.5	94.19	90.87				
60%	98.08	104.77	101.45				

#### APPENDIX C.1

#### ESTIMATION OF PRODUCT COST FOR CONVENTIONAL POLYSILICON PROCESS: CASE C

		PRODUCT COST, \$/KG Si									
		LOW 1.8¢/KW.HR	HIGH 3.6¢/KW.HR	INTERMED. 2.7¢/KW.HR							
1.	Direct Manufacturing Cost (Direct Cost) 1. Raw Materials 2. Direct Operating Labor 3. Utilities 4. Supervision and Clerical	16.87 4.02 9.64 .60	16.87 4.02 16.56 .60	16.87 4.02 13.10 .60							
	<ol> <li>Maintenance and Repairs</li> <li>Operating Supplies</li> <li>Laboratory Charge</li> </ol>	2.38 .48 .60	2.38 .48 .60	2.38 .48 .60							
2.	Indirect Manufacturing Cost (Fixed Cost) 1. Depreciation 2. Local Taxes 3. Insurance	 .92 .46	 .92 .46	 .92 .46							
3.	Plant Overhead	4.20	4.20	4.20							
4.	By-Product Credit	(6.85)	(6.85)	(6.85)							
4a.	Total Manufacturing Cost, $1 + 2 + 3 + 4$	33.32	40.24	36.78							
5.	General Expenses 1. Administration 2. Distribution and Sales 3. Research and Development	2.00 2.00 1.00	2.41 2.41 1.21	2.21 2.21 1.10							
6.	Product Cost Without Profit, 4a + 5	38.32	46.27	42.30							
7.	Profit For Product (After Taxes)										

8. Product Cost With Profit, 6 + 7

Basis: Case C is based on 1977 costs for plant constructed in 1960's. Most plants producing polysilicon in U.S.A. were constructed in 1960's or earlier. Range reflects low and high electrical costs (1.5-3¢/KW.HR plus 20% escalation). Intermediate reflects intermediate electrical cost (2.25¢/KW.HR plus 20% escalation).

# APPENDIX C.2

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PRODUCT COST VARIATION (SALES PRICE) WITH RETURN ON INVESTMENT (ROI): CASE C

•	ProcessC	Conventional Polysilicon Process
•	Plant Sizel	,000 Metric Tons/Year
•	Plant ProductS	Semiconductor Grade Polysilicon
•	Plant Investment\$	52,900,000

	PRODUCT COST WITH PROFIT:									
	SALES PRICE, \$/KG Si									
RETURN ON INVESTMENT AFTER TAXES &ROI	LOW 1.8¢/KW.HR	HIGH 3.6¢/KW.HR	INTERMED. 2.7¢/KW.HR							
0	38.32	46.27	42.30							
5%	43.61	51.56	47.59							
10%	48.90	56.85	52.88							
15%	54.19	62.14	58.17							
20%	59.48	67.43	63.46							
25%	64.77	72.72	68.75							
30%	70.06	78.01	74.04							
40%	80.64	88.59	84.62							
50%	91.22	99.17	95.20							
60%	101.80	109.75	105.78							

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System Properties																								
1, Prel. Data Collection																								
2.Data Analysis		Ì																						
3, Estimation Methods																								
4, ExpCorr. Activities																								
5, Prel. Prop. Values																								
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1.Prel. Process Flow Diag.																								
2.Reaction Chemistry																								
3.Kinetic Rate Data																								
4.Major Equip. Req.																								
5.Chem. EquilExp. Act.																							- 14 - 14	
6, Process Comparison																								
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l.Cap. Invest. Est.																								
2.Raw Materials																								
3.Utilities	_																							
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Final Report		ţ																						

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PROCESS FEASIBILITY STUDY IN SUPPORT OF SILICON MATERIAL TASK I

JPL Contract No. 954343

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