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PROCESS FEASIBILITY STUDY IN SUPPORT OF  
SILICON MATERIAL TASK I

Quarterly Technical Progress Report (VI)

March, 1977

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IN SUPPORT OF SILICON MATERIAL TASK I  
Quarterly Technical Progress Report (Lamar  
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## ABSTRACT

During this reporting period, major efforts were expended on process system properties, chemical engineering and economic analyses.

In Task 1, major activities were continued on process system properties of silicon source materials under consideration for solar cell grade silicon production. In property correlation efforts, property data results are presented for heat of vaporization, gas heat capacity, liquid heat capacity, liquid density, surface tension and gas viscosity of silane ( $\text{SiH}_4$ ) as a function of temperature.

The correlation results for gas heat capacity covers both low and high temperature ranges which will be encountered (low temperature range-silane production, high temperature range - silicon production from silane) in the specific process technology. These results will be used in the performance of the chemical engineering analysis of the silane process (Union Carbide).

Major chemical engineering analysis activities in Task 2 are being devoted to preliminary process design for a silane ( $\text{SiH}_4$ ) plant that will produce 1000 metric tons/year of solar cell grade silicon. The technology developed by Union Carbide for the production of silane uses hydrogen and metallurgical grade silicon as raw materials. Preliminary process flow diagram and base conditions are reported. In addition for the flow diagram as initially received, technical interchange was initiated in regards to several material balance closures and operating conditions. A revised flow-sheet from Union Carbide discussing the same has just been received for review.

For Task 2, preliminary process design was initiated for the conventional polysilicon process now used in the United States to produce semiconductor grade silicon from TCS (trichlorosilane,  $\text{SiHCl}_3$ ).

Economic analysis activities in Task 3 focused on development of a computer model to aid in estimation of product and plant investment costs for the alternate solar cell grade silicon processes. Application of the computer model to the Battelle process ( $\text{Zn/SiCl}_4$ ) indicated \$10,510,000 fixed capital investment and \$9.63/KG of silicon for a 1000 metric ton/yr. plant.

Economic analysis activities also centered on developing cost standardization techniques for application to the alternate processes. These techniques and information presented will allow valid comparisons between processes on a standardized basis.

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

Major efforts were continued on process system properties of silicon source materials. Additional correlation efforts were expended on property data required in the performance of the chemical engineering analyses of the alternate processes under consideration for solar cell grade silicon production.

Heat of vaporization data for silane are available only at the boiling point (A2, A21, A22, A23, A27, A41). These data vary less than 1%. Watson's correlation (A27, A29) was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_V = \Delta H_{V_1} \left( \frac{T_C - T}{T_C - T_1} \right)^n \quad (I-1)$$

where  $\Delta H_{V_1}$  is the heat of vaporization at the boiling point and  $n = .38$ .

Figure I-1 presents results for heat of vaporization versus temperature for silane.

For silane, heat capacity data of the ideal gas at low pressure are primarily based on structural and spectral measurements. Values from the various sources (A5, A16, A20, A22, A25, A39, A44, A52) are in excellent agreement. The data were correlated by a series expansion in temperature:

$$C_P = A + BT + CT^2 + DT^3 \quad (I-2)$$

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

The correlation constants ( $A$ ,  $B$ ,  $C$  and  $D$ ) 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.

Correlation values and data are in close agreement with average deviations of only 0.5%. The correlation covers both low temperature (region for silane production) and high temperature (region for silicon production from silane) ranges. Figure I-2 presents results for gas phase heat capacity of silane.

Liquid heat capacity results from silane are given in Figure I-3. Liquid heat capacity data (A6) are available in the mp-bp temperature interval. The data were extended to cover the full liquid phase with the density relation: liquid heat capacity x density = constant. The constant value was 0.29.

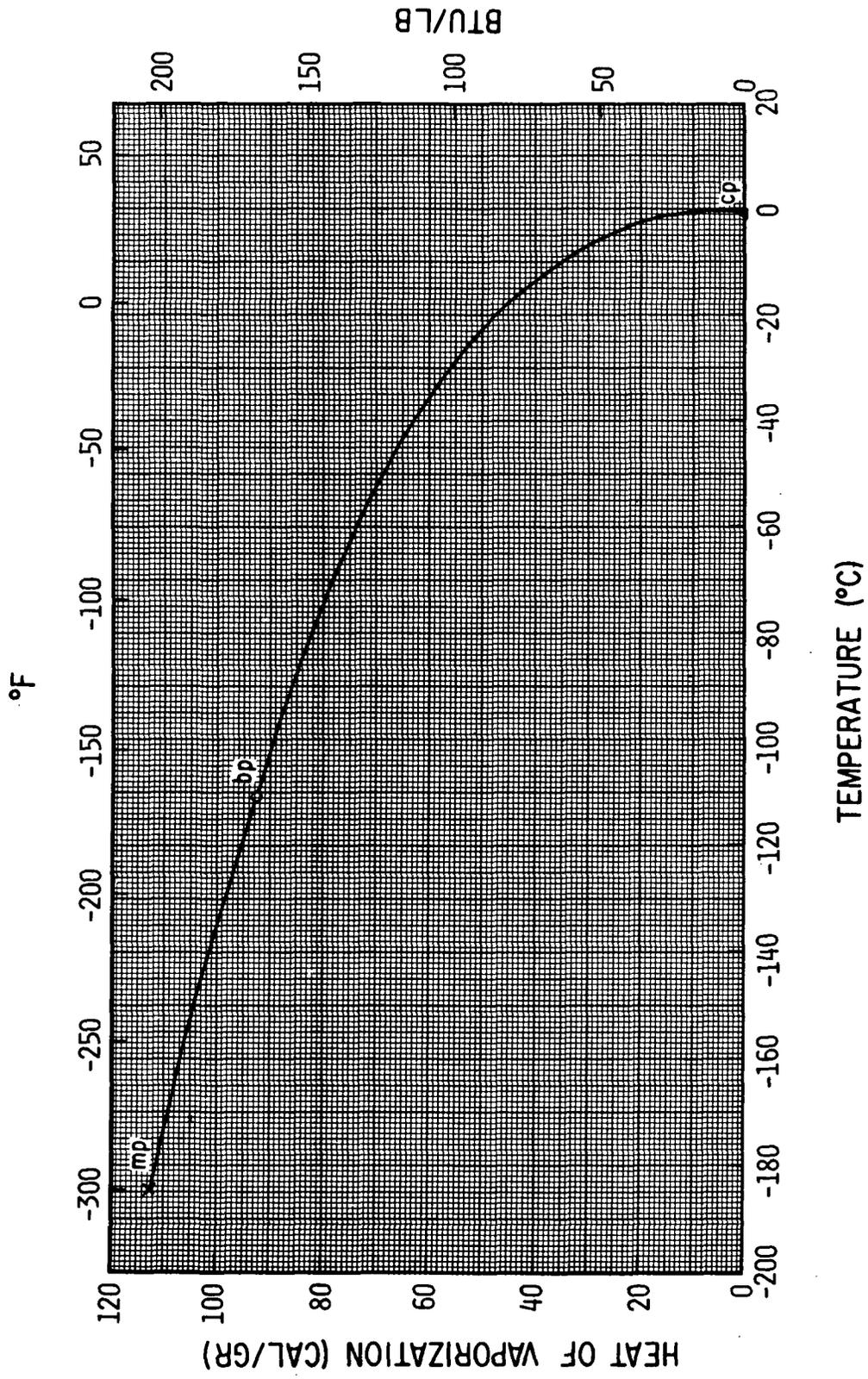


Figure I-1 Heat of Vaporization Vs. Temperature for Silane

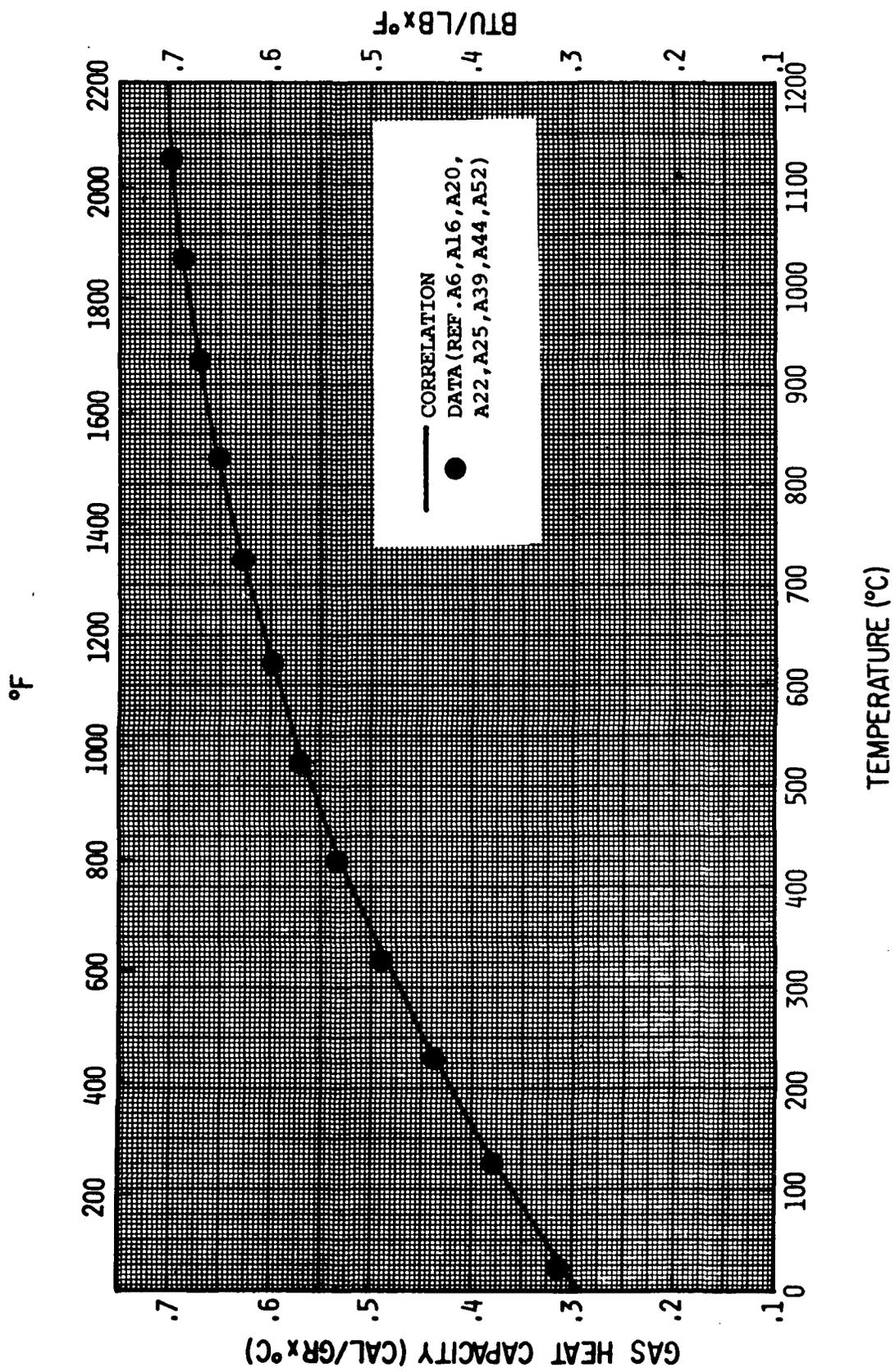


Figure I-2 Gas Heat Capacity Vs. Temperature for Silane

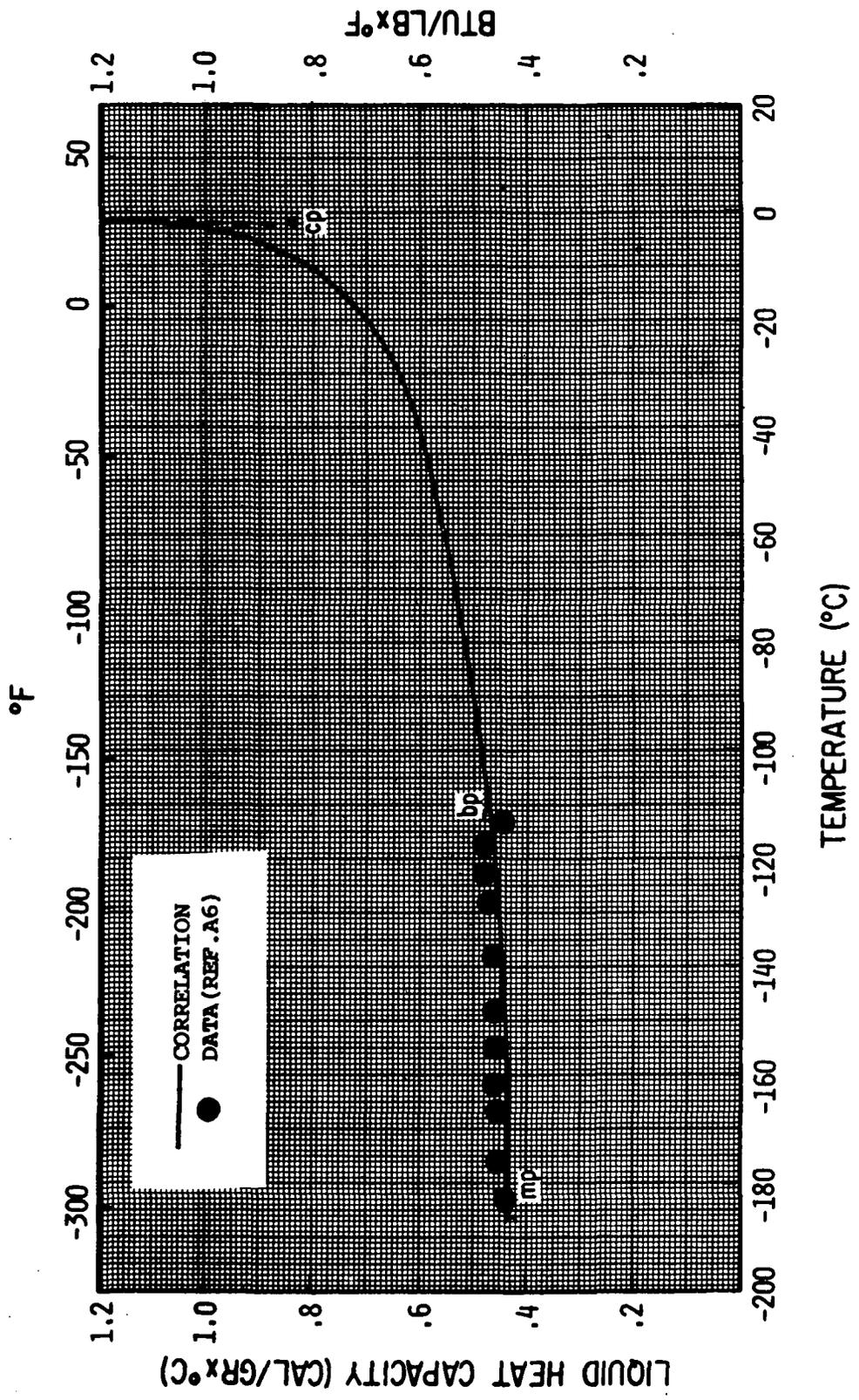


Figure I-3 Liquid Heat Capacity Vs. Temperature for Silane

Liquid density data for silane are available (A2, A15, A18, A23, A25, A35, A48, A52) from the melting point to the boiling point. The Yaws-Shah equation (A62) for density of the saturated liquid was used to extend the data to the critical point:

$$\rho = A B^{-(1-T_r)^{2/7}} \quad (I-3)$$

where:  $\rho$  = density, g/cm<sup>3</sup>,  $T_r$  = reduced temperature,  $T/T_c$ , A, B = correlation parameters. The correlation parameter values for silane are A = 0.2447 and B = 0.3137. Average deviation of calculated values and experimental data is 1.48%. Results for liquid density versus temperature are shown in Figure I-4.

Data for surface tension (A7) are available from the melting point to the boiling point. These data were extended using the Othmer relation (A29):

$$\sigma = \sigma_1 \left[ \frac{T_c - T}{T_c - T_1} \right]^n \quad (I-4)$$

where  $\sigma_1$  = surface tension at  $T_1$ , dynes/cm;  $T_c$  = critical temperature, °K;  $T$  = temperature, °K; and  $n$  = the correlation parameter, 1.2. Deviations between data and correlated values were less than 1%. Figure I-5 shows surface tension results for silane.

Gas viscosity data for silane are lacking for the most part. Two experimental data points are available at temperatures of 15°C and 100°C from the work of Rankine (A57) who made the measurements in 1922. Some sources cite a third data point at 0°C, but this is really an extrapolated-calculated value from the original Rankine paper. Additional data are needed, especially at higher temperatures which will be encountered in silicon deposition.

The Stiel and Thodos correlation (A29) was used to augment the limited data on gas viscosity (A2, A15, A20, A21, A23, A25, A52, A53, A57) at atmospheric pressure:

$$\mu_G = \frac{z}{\epsilon}^{-5/4} \left[ 0.755 Tr - 0.055 \right] \quad (I-5)$$

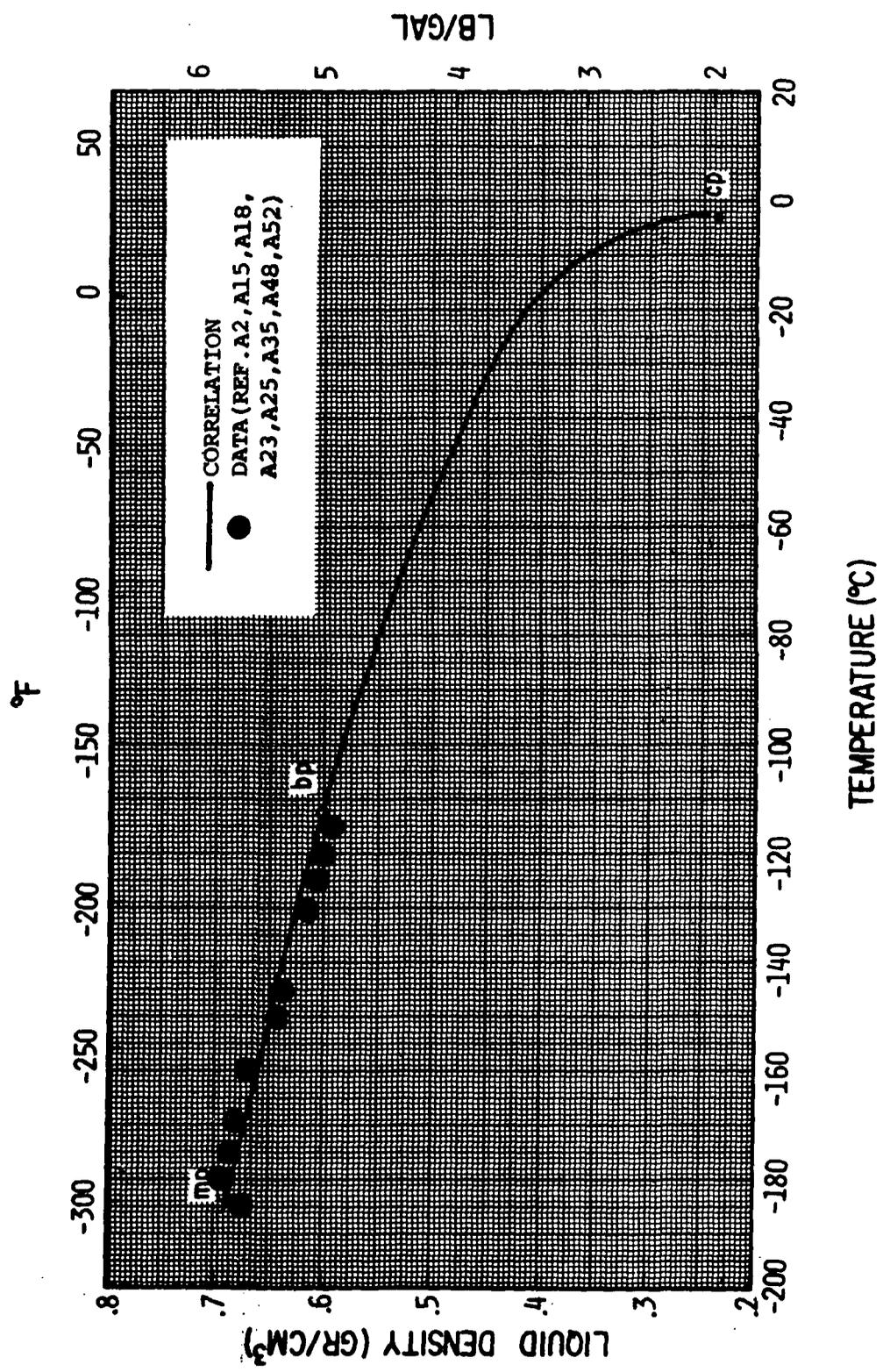


Figure I-4 Liquid Density Vs. Temperature for Silane

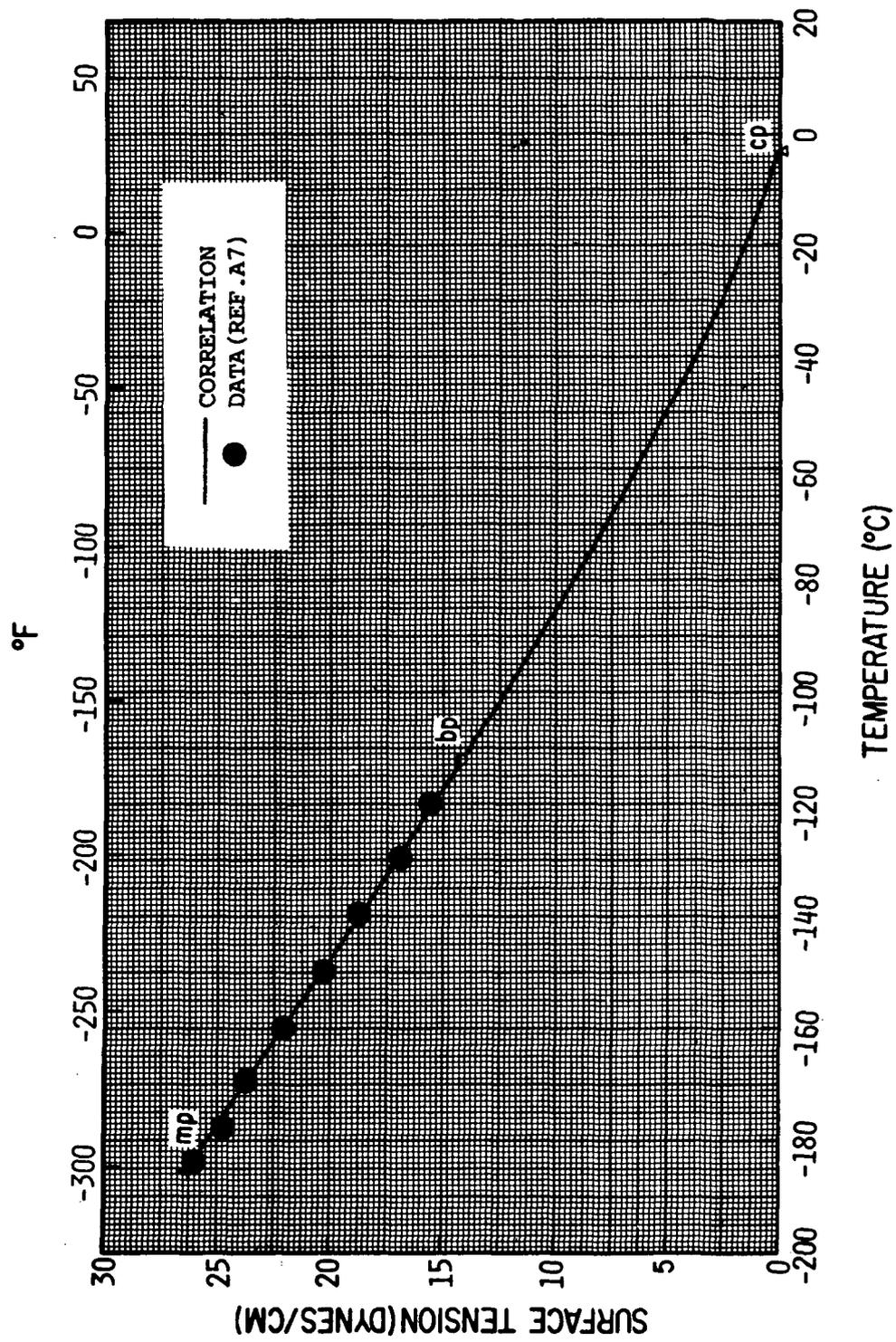


Figure I-5 Surface Tension Vs. Temperature for Silane

where:  $\mu_G$  = gas viscosity at low pressure (1 atm), micropoise,  
 $\epsilon$  = correlation parameter,  $Z_c$  = critical compressibility factor and  
 $T_r$  = reduced temperature,  $T/T_c$ . All data sources cite Rankine (A57).  
Deviations between data and correlation were less than 1.0% for the  
two data values.

Results are presented in Figure I-6 which displays gas viscosity of  
silane versus temperature. Both metric units (micropoise) and conven-  
tional engineering units (lb/ft x sec) are given in the plot. The plot  
may be used in important engineering calculations such as the Prandtl  
( $C_p \mu/k$ ) and Reynolds ( $Du\rho/\mu$ ) numbers which are important in characterizing  
fluidized bed behavior.

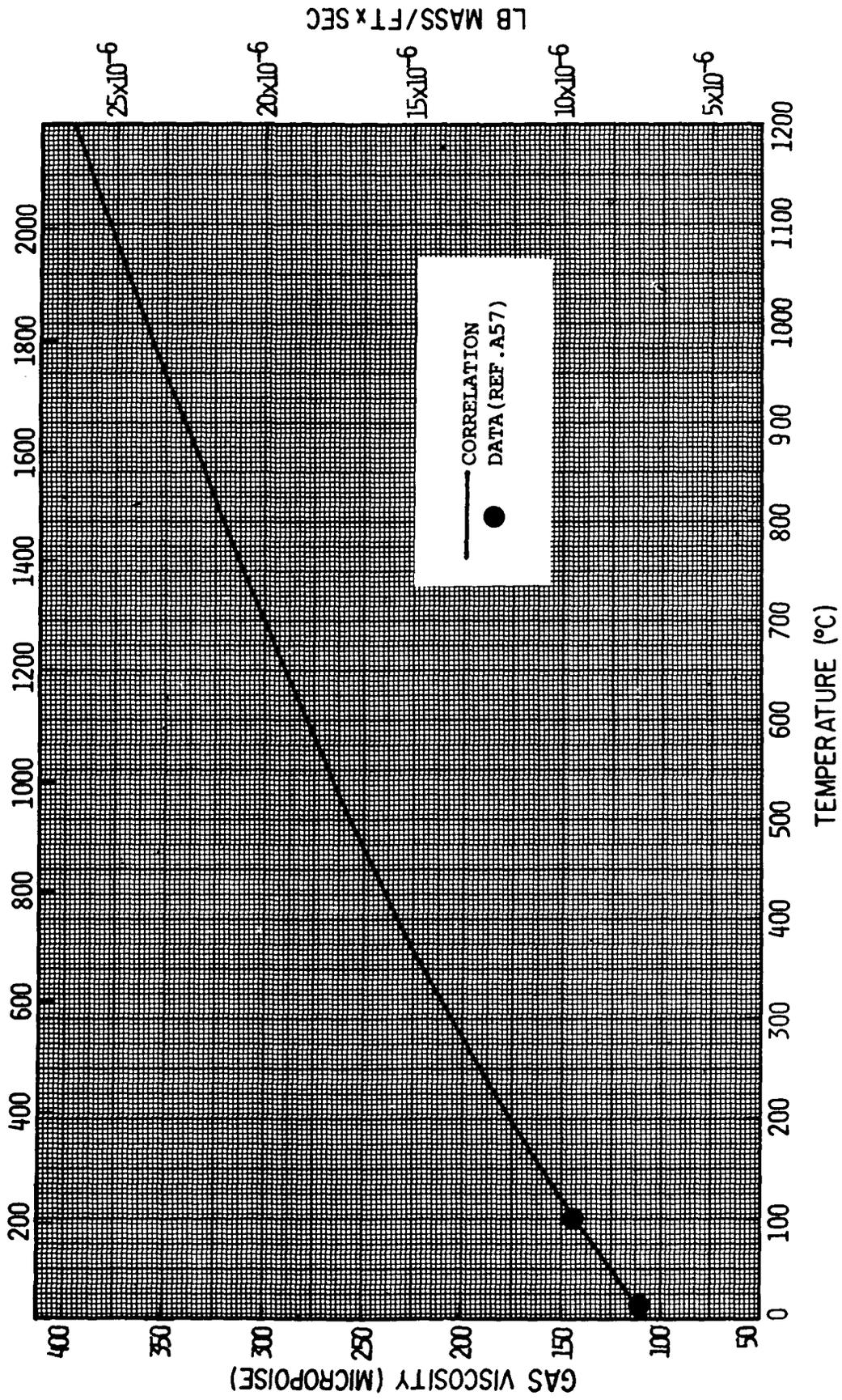


Figure I-6 Gas Viscosity Vs Temperature for Silane

## II. CHEMICAL ENGINEERING ANALYSES (TASK 2)

### A. Silane Process (Union Carbide)

Chemical engineering analyses were continued during this reporting period for alternate processes under consideration for solar cell grade silicon.

Major efforts are being directed toward the preliminary process design for the silane process (Union Carbide). The status, including progress since the last reporting period for the process design is given below for key guideline items:

|                      | <u>Current</u> |
|----------------------|----------------|
| Process Flow Diagram | 60%            |
| Material Balance     | 15%            |
| Energy Balance       | 0%             |
| Property Data        | 40%            |
| Equipment Design     | 0%             |

The status, including activities accomplished, in progress, and planned are shown in Table IIA-1 for the preliminary process design. The preliminary process flow sheet as initially received from Union Carbide is given in Figure IIA-1.

The partial results of the preliminary process design are summarized in a tabular format. The guide for the primary results in the accompanying tables is given below:

|                           |             |
|---------------------------|-------------|
| Base Case Conditions..... | Table IIA-2 |
| Reaction Chemistry.....   | Table IIA-3 |

The Base Case Conditions are summarized in Table IIA-2, production capacity set at the amount of silane necessary to produce 1000 metric tons/year of solar cell grade silicon. The relatively high value of the utility (90%) was chosen because of the low pressures and temperatures involved. Raw materials are metallurgical grade silicon and hydrogen which are reacted with by-product silicon tetrachloride to produce trichlorosilane which is redistributed in two stages with tertiary amine ion exchange resin. Product silane from the redistribution reactions is purified in two-stages by absorption with cold (-40°C) silicon tetrachloride and activated carbon adsorption.

Table IIA-3 and Figure IIA-2 represents the reaction chemistry for the process. The hydrogenation reaction is catalyzed in a fluidized bed with copper at 550°C, 50 PSIG. Figure IIA-2 is related to both of the redistribution reactions and gives the equilibrium mix of chlorosilanes as a function of the chlorine to silicon ratio in the inlet stream. This figure was obtained from Union Carbide.

TABLE IIA-1 CHEMICAL ENGINEERING ANALYSES:  
 PRELIMINARY PROCESS DESIGN ACTIVITIES FOR SILANE PROCESS (UNION CARBIDE)

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



TABLE IIA-2

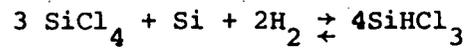
BASE CASE CONDITIONS FOR SILANE PROCESS (Union Carbide)

1. Plant Size
  - Allow for 10% losses of silane in production of silicon
  - 1270 metric tons/year
  - Solar cell grade silicon
2. Hydrogenation Reaction
  - Metallurgical grade silicon and hydrogen to produce trichlorosilane (TCS)
  - Copper catalyzed
  - Fluidized bed
  - 550°C, 50 PSIG
  - 15.8% conversion of  $\text{SiCl}_4$  (Union Carbide flowsheet)
3. TCS Redistribution Reaction
  - TCS from hydrogenation produces dichlorosilane (DCS)
  - Catalytic redistribution of TCS with tertiary amine ion exchange resin.
  - Liquid phase 50 PSIG, 80°C.
  - Conversion a function of inlet concentration per Figure IIA-2 (Union Carbide equilibrium)
4. DCS Redistribution Reaction
  - DCS produces  $\text{SiH}_4$  (silane)
  - Catalytic redistribution of DCS with tertiary amine ion exchange resin.
  - Gas phase 60-80°C
  - Conversion a function of inlet concentration per Figure IIA-2 (Union Carbide equilibrium)
5. Recycles
  - Unreacted chlorosilanes separated by distillation and recycled
6. Silane Purification
  - Chlorosilanes removed by absorption in -40°C  $\text{SiCl}_4$  (Tet)
  - Trace contaminants removed by carbon adsorption
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)

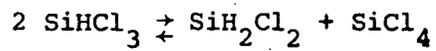
TABLE IIA-3

REACTION CHEMISTRY

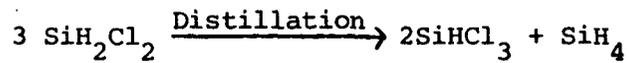
1. Hydrogenation Reaction



2. Trichlorosilane Redistribution Reaction



3. Dichlorosilane Redistribution Reaction



Note

1. Reaction 1 Product contains  $\text{H}_2$ ,  $\text{SiCl}_4$ ,  $\text{SiHCl}_3$ ,  $\text{SiH}_2\text{Cl}_2$  (trace), other trace chlorides
2. Reaction 2 Product contains  $\text{SiHCl}_3$ ,  $\text{SiCl}_4$ ,  $\text{SiH}_2\text{Cl}_2$ ,  $\text{SiH}_3\text{Cl}$
3. Reaction 3 Product contains  $\text{SiH}_2\text{Cl}_2$ ,  $\text{SiHCl}_3$ ,  $\text{SiCl}_4$ ,  $\text{SiH}_3\text{Cl}$ ,  $\text{SiH}_4$

SIZE 10 X 10 TO 12 INCH 46 1432  
 1 1/2 X 1/2 5 INCHES  
 KEUFFEL & ESSER CO.

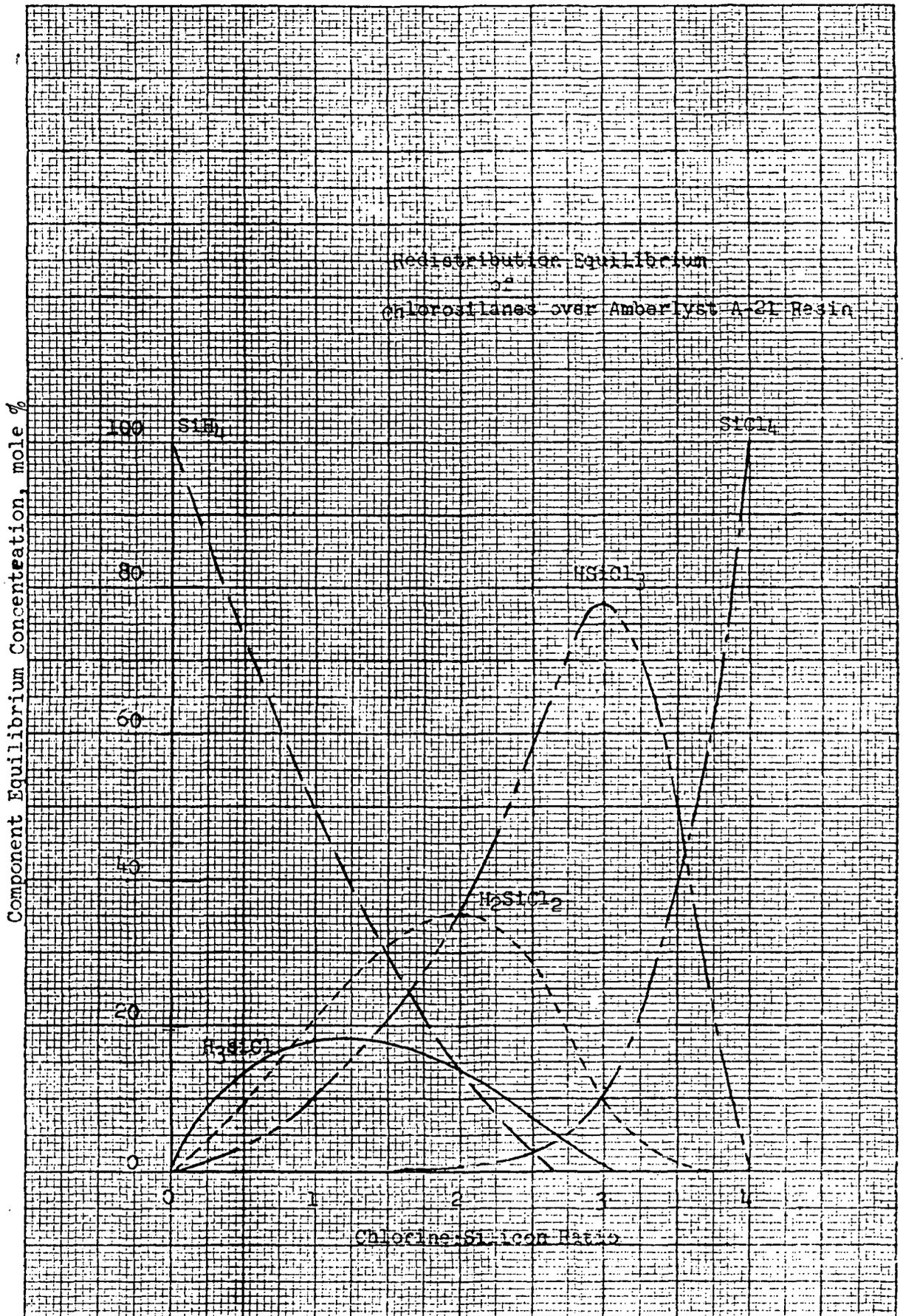


Figure IIA-2 Redistribution Equilibrium For Silane Process  
 (Provided by Union Carbide)

For the process flow diagram as initially received, technical interchange was initiated with Union Carbide in regards to several material balance closures and operating conditions necessary for performance of the chemical engineering analyses. A revised flow-sheet discussing material balance closure and appropriate operating conditions has just arrived from Union Carbide. This revised flow-sheet will be reviewed and used for performing the preliminary process design of the silane process.

## B. Conventional Polysilicon Process.

Major efforts are being directed toward the preliminary process design for the conventional polysilicon process now used in the United States for the production of semiconductor grade silicon from TCS (trichlorosilane,  $\text{SiHCl}_3$ ). In this process, metallurgical grade silicon and HCl gas are reacted in a fluidized bed reactor to make TCS which is purified in a complex distillation process. The purified TCS is reduced with hydrogen at high temperature ( $>1000^\circ\text{C}$ ) over heated filaments (rods) to produce silicon.

Information on the process is being obtained from the open literature (20, 31, 32) and from Dr. Leon Crossman of Dow Chemical Company. The rationale for the design and economic evaluation of an existing production facility is to verify the methodology currently utilized for proposed technologies.

The status for the preliminary process design, including status since the last reporting period is given below for key guideline items:

|                      | <u>Prior</u> | <u>Current</u> |
|----------------------|--------------|----------------|
| Process Flow Diagram | 0%           | 50%            |
| Material Balance     | 0%           | 30%            |
| Energy Balance       | 0%           | 0%             |
| Property Data        | 0            | 0%             |
| Equipment Design     | 0%           | 15%            |

The status, including activities accomplished, in progress, and planned are shown in Table IB-1 for the preliminary process design.

TABLE IIB-1 CHEMICAL ENGINEERING ANALYSES:  
PRELIMINARY PROCESS DESIGN ACTIVITIES FOR CONVENTIONAL POLYSILICON PROCESS

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

0 Plan  
● In Progress  
● Complete

### III. ECONOMIC ANALYSES (TASK 3)

#### A. Cost Standardization Considerations

Certain considerations effecting the final product cost are being standardized so that economic analyses made for various processes will reflect valid comparisons. The base case conditions for preliminary process design and economic analyses are summarized in Table IIIA-1. The base case conditions includes cost standardization considerations with respect to plant size, storage considerations, capital investment, raw material cost, utilities and labor cost.

Standardized utility costs are given in Table IIIA-2 for application to the various processes. Utility costs fluctuate a great deal with location and time. The recent natural gas shortage and the rising oil prices serve to make these numbers more subject to change as time goes by. However, the tabulated data do reflect reasonable values for 1975.

TABLE IIIA-1

COST STANDARDIZATION CONSIDERATIONS: BASE CASE CONDITIONS

1. Plant Size
  - Production of 1000 metric tons/year
  - Solar Cell Grade Silicon
2. Storage Considerations
  - Feed materials (two week supply)
  - Product (two week supply)
  - Process (several days)
3. Capital Equipment
  - Jan. 1975 Cost Index for Capital Equipment Cost (M and S Index)
  - Jan. 1975 Cost Index Value = 430
4. Raw Material Cost
  - Chemical Marketing Report
  - Jan. 1975 Value
5. Utilities
  - Electrical, Heating, Cooling, Etc.
  - Jan. 1975 Cost Index (U.S. Dept. Labor)
  - Value = 181 (1967 Base = 100)
6. Labor Cost
  - Average for Chemical, Petroleum, Coal and Allied Industries (1975)
  - Skilled 6.90 \$/hr
  - Semiskilled 4.90 \$/hr

TABLE IIIA-2

## COST STANDARDIZATION: UTILITY COSTS\*

| <u>ITEM</u>               | <u>PRICE</u>            |
|---------------------------|-------------------------|
| 1. Fuel (oil)             | \$1.55/MM BTU           |
| 2. Steam                  | \$1.25/M LB             |
| 3. Cooling Tower Water    | \$.08/M GAL             |
| 4. Process Water          | \$.35/M GAL             |
| 5. Electricity            | 3¢/KW HR                |
| 6. Compressed Air         | \$.35/M CU FT (S.T.P.)  |
| 7. Refrigeration to 34°F  | \$3.75/MM BTU           |
| 8. Refrigeration to -20°F | \$8.68/MM BTU           |
| 9. Natural Gas            | \$1.25/M CU FT (S.T.P.) |
| 10. Nitrogen              | \$.50/M CU FT (S.T.P.)  |

NOTE

M = 1000  
MM = 1,000,000

\*Values taken from references 1,5,6,11,7,13,22,26,29 and 30.  
Applicable for 1975 time period.

## B. Computer Model

Economic analyses activities were continued in the development of a computer model to aid in the cost evaluation of alternate processes under consideration for solar cell grade silicon.

Primary initial activities were devoted to development of the computer model for use in estimation of plant investment cost. In the computer model, the plant investment (fixed capital) is determined from direct plant investment costs (major process equipment cost, installation, process piping, instrumentation, electrical and process buildings); other direct plant investment costs (utilities, general services such as site development and fire protection, general buildings such as offices and shops and receiving-shipping facilities); indirect plant investment costs (such as engineering and normal cont. for material delays, labor problems, etc.) and overall contingency.

After preliminary debugging, the computer model was applied to the Zn/SiCl<sub>4</sub> process (Battelle). Preliminary process design data from the chemical engineering analysis activity were used in the computer model including major process equipment, raw materials, utilities and labor requirements. Results for estimation of plant investment cost are shown in Table IIIB-1. Table IIIB-2 presents results for the product cost.

The cost evaluation results from the computer model indicate \$10,510,000 fixed capital investment and \$9.63/KG of silicon for the Zn/SiCl<sub>4</sub> process (Battelle). These cost estimates apply to a 1000 metric ton/yr plant size.

The computer model was then applied to the Zn/SiCl<sub>4</sub> process (Battelle technology) at three levels of plant investment (\$5, \$10 and \$15 million). Results are given in Tables IIIB-3, IIIB-4 and IIIB-5 for the cost change items. Estimated total product costs are \$7.27, 9.42 and \$11.56/KG of silicon at each respective plant investment level.

## ECONOMIC ANALYSIS

## ZN/SICL4 PROCESS BATTELLE

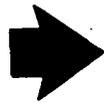
 ESTIMATION OF PLANT INVESTMENT

|  | PER CENT OF<br>EQUIPMENT<br>COST | INVESTMENT,<br>THOUSANDS<br>OF DOLLARS |
|--|----------------------------------|--|
| 1. DIRECT PLANT INVESTMENT COSTS   |                                  |  |
| 1. MAJOR PROCESS EQUIPMENT COST  | 100.0                            | 1977.                                  |
| 2. INSTALLATION OF MAJOR PROCESS EQUIPMENT   | 42.0                             | 830.                                   |
| 3. PROCESS PIPING, INSTALLED   | 45.0                             | 890.                                   |
| 4. INSTRUMENTATION, INSTALLED  | 14.0                             | 277.                                   |
| 5. ELECTRICAL, INSTALLED   | 9.0                              | 178.                                   |
| 6. PROCESS BUILDINGS, INSTALLED  | 8.0                              | 158.                                   |
| 1A. SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS<br>(PRIMARILY BATTERY LIMIT FACILITIES) |                                  | 4310.                                  |
| 2. OTHER DIRECT PLANT INVESTMENT COSTS   |                                  |  |
| 1. UTILITIES, INSTALLED  | 34.0                             | 672.                                   |
| 2. GENERAL SERVICES, SITE DEVELOPMENT,<br>FIRE PROTECTION, ETC.                        | 16.0                             | 316.                                   |
| 3. GENERAL BUILDINGS, OFFICES, SHOPS, ETC.   | 21.0                             | 415.                                   |
| 4. RECEIVING, SHIPPING FACILITIES  | 21.0                             | 415.                                   |
| 2A. SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS<br>(PRIMARILY OFFSITE FACILITIES) |                                  | 1819.                                  |
| 3. TOTAL DIRECT PLANT INVESTMENT COST, 1A + 2A   |                                  | 6129.                                  |
| 4. INDIRECT PLANT INVESTMENT COSTS   |                                  |  |
| 1. ENGINEERING, OVERHEAD, ETC.   | 44.0                             | 870.                                   |
| 2. NORMAL CONT. FOR FLOODS, STRIKES, ETC.  | 55.0                             | 1087.                                  |
| 4A. TOTAL INDIRECT PLANT INVESTMENT COST   |                                  | 1957.                                  |
| 5. TOTAL DIRECT AND INDIRECT PLANT INVESTMENT<br>COST, 3 + 4A                          |                                  | 8086.                                  |
| 6. OVERALL CONTINGENCY, PER CENT OF 5  | 30.0                             | 2426.                                  |
| 7. TOTAL PLANT INVESTMENT (FIXED CAPITAL),<br>5 + 6                                    |                                  | 10512. <i>new.</i>                     |



## ECONOMIC ANALYSIS

## ZN/SICL4 PROCESS BATTELLE



## ESTIMATION OF TOTAL PRODUCT COST

|  | COST,<br>DOLLARS/KG PROD. |
|--|---------------------------|
| 1. DIRECT MANUFACTURING COST (DIRECT CHARGES)  |                           |
| 1. RAW MATERIALS - FROM PREL. DESIGN   | 2.76                      |
| 2. DIRECT OPERATING LABOR - FROM PREL. DESIGN  | 0.52                      |
| 3. UTILITIES - FROM PREL. DESIGN   | 0.88                      |
| 4. SUPERVISION AND CLERICAL, 15.00 PER CENT OF 1.2   | 0.08                      |
| 5. MAINTENANCE AND REPAIRS, 10.00 PER CENT OF FIXED CAPITAL (50 PER CENT LABOR, 50 PER CENT MATERIALS) | 1.05                      |
| 6. OPERATING SUPPLIES, 20.00 PER CENT OF 1.5   | 0.21                      |
| 7. LABORATORY CHARGE, 15.00 PER CENT OF 1.2  | 0.08                      |
| 8. PATENTS AND ROYALTIES, 3.00 PER CENT OF PROD. COST  | 0.29                      |
| 2. INDIRECT MANUFACTURING COST (FIXED CHARGES)   |                           |
| 1. DEPRECIATION, 10.00 PER CENT OF FIXED CAPITAL   | 1.05                      |
| 2. LOCAL TAXES, 2.00 PER CENT OF FIXED CAPITAL   | 0.21                      |
| 3. INSURANCE, 1.00 PER CENT OF FIXED CAPITAL   | 0.11                      |
| 4. INTEREST, 8.00 PER CENT OF FIXED CAPITAL  | 0.84                      |
| 3. PLANT OVERHEAD, 60.00 PER CENT OF LABOR IN 1.2+1.4+1.5  | 0.67                      |
| 4. BY-PRODUCT CREDIT - FROM PREL. DESIGN   | -0.37                     |
| 4A. TOTAL MANUFACTURING COST, 1 + 2 + 3 + 4  | 8.38                      |
| 5. GENERAL EXPENSES  |                           |
| 1. ADMINISTRATION, 6.00 PER CENT OF MANUF. COST  | 0.50                      |
| 2. DISTRIBUTION AND SALES, 6.00 PER CENT OF MANUF. COST  | 0.50                      |
| 3. RESEARCH AND DEVELOPMENT, 3.00 PER CENT OF MANUF. COST  | 0.25                      |
| 6. TOTAL COST OF PRODUCT, 4A + 5   | 9.63 <i>rev.</i>          |

PLANT INVESTMENT (FIXED CAPITAL), 10.51 MILLION DOLLARS

TABLE IIIB-3

ECONOMIC ANALYSIS  
 ZN/SICL<sub>4</sub> PROCESS BATTELLE  
 ESTIMATION OF TOTAL PRODUCT COST

|  | COST,<br>DOLLARS/KG PROD. |
|--|---------------------------|
| 1. DIRECT MANUFACTURING COST (DIRECT CHARGES)  |                           |
| 1. RAW MATERIALS                               | 2.76                      |
| 2. DIRECT OPERATING LABOR                      | 0.52                      |
| 3. UTILITIES                                   | 0.88                      |
| 4. SUPERVISION AND CLERICAL                    | 0.08                      |
| 5. MAINTENANCE AND REPAIRS                     | 0.50                      |
| 6. OPERATING SUPPLIES                          | 0.10                      |
| 7. LABORATORY CHARGE                           | 0.08                      |
| 8. PATENTS AND ROYALTIES                       | 0.22                      |
| 2. INDIRECT MANUFACTURING COST (FIXED CHARGES) |                           |
| 1. DEPRECIATION                                | 0.50                      |
| 2. LOCAL TAXES                                 | 0.10                      |
| 3. INSURANCE                                   | 0.05                      |
| 4. INTEREST                                    | 0.40                      |
| 3. PLANT OVERHEAD                              | 0.51                      |
| 4. BY-PRODUCT CREDIT                           | -0.37                     |
| 4A. TOTAL MANUFACTURING COST, 1 + 2 + 3 + 4    | 6.32                      |
| 5. GENERAL EXPENSES                            |                           |
| 1. ADMINISTRATION                              | 0.38                      |
| 2. DISTRIBUTION AND SALES                      | 0.38                      |
| 3. RESEARCH AND DEVELOPMENT                    | 0.19                      |
| 6. TOTAL COST OF PRODUCT, 4A + 5               | 7.27                      |

PLANT INVESTMENT (FIXED CAPITAL), 5.00 MILLION DOLLARS

TABLE IIIB-4

ECONOMIC ANALYSIS  
 ZN/SICL<sub>4</sub> PROCESS BATTELLE  
 ESTIMATION OF TOTAL PRODUCT COST

|  | COST,<br>DOLLARS/KG PROD. |
|--|---------------------------|
| 1. DIRECT MANUFACTURING COST (DIRECT CHARGES)  |                           |
| 1. RAW MATERIALS                               | 2.76                      |
| 2. DIRECT OPERATING LABOR                      | 0.52                      |
| 3. UTILITIES                                   | 0.88                      |
| 4. SUPERVISION AND CLERICAL                    | 0.08                      |
| 5. MAINTENANCE AND REPAIRS                     | 1.00                      |
| 6. OPERATING SUPPLIES                          | 0.20                      |
| 7. LABORATORY CHARGE                           | 0.08                      |
| 8. PATENTS AND ROYALTIES                       | 0.28                      |
| 2. INDIRECT MANUFACTURING COST (FIXED CHARGES) |                           |
| 1. DEPRECIATION                                | 1.00                      |
| 2. LOCAL TAXES                                 | 0.20                      |
| 3. INSURANCE                                   | 0.10                      |
| 4. INTEREST                                    | 0.80                      |
| 3. PLANT OVERHEAD                              | 0.66                      |
| 4. BY-PRODUCT CREDIT                           | -0.37                     |
| 4A. TOTAL MANUFACTURING COST, 1 + 2 + 3 + 4    | 8.19                      |
| 5. GENERAL EXPENSES                            |                           |
| 1. ADMINISTRATION                              | 0.49                      |
| 2. DISTRIBUTION AND SALES                      | 0.49                      |
| 3. RESEARCH AND DEVELOPMENT                    | 0.25                      |
| 6. TOTAL COST OF PRODUCT, 4A + 5               | 9.42                      |

PLANT INVESTMENT (FIXED CAPITAL), 10.00 MILLION DOLLARS

TABLE IIIB-5

## ECONOMIC ANALYSIS

## ZN/SICL4 PROCESS BATTELLE

## ESTIMATION OF TOTAL PRODUCT COST

|  | COST,<br>DOLLARS/KG PROD. |
|--|---------------------------|
| 1. DIRECT MANUFACTURING COST (DIRECT CHARGES)  |                           |
| 1. RAW MATERIALS                               | 2.76                      |
| 2. DIRECT OPERATING LABOR                      | 0.52                      |
| 3. UTILITIES                                   | 0.88                      |
| 4. SUPERVISION AND CLERICAL                    | 0.08                      |
| 5. MAINTENANCE AND REPAIRS                     | 1.50                      |
| 6. OPERATING SUPPLIES                          | 0.30                      |
| 7. LABORATORY CHARGE                           | 0.08                      |
| 8. PATENTS AND ROYALTIES                       | 0.35                      |
| 2. INDIRECT MANUFACTURING COST (FIXED CHARGES) |                           |
| 1. DEPRECIATION                                | 1.50                      |
| 2. LOCAL TAXES                                 | 0.30                      |
| 3. INSURANCE                                   | 0.15                      |
| 4. INTEREST                                    | 1.20                      |
| 3. PLANT OVERHEAD                              | 0.81                      |
| 4. BY-PRODUCT CREDIT                           | -0.37                     |
| 4A. TOTAL MANUFACTURING COST, 1 + 2 + 3 + 4    | 10.05                     |
| 5. GENERAL EXPENSES                            |                           |
| 1. ADMINISTRATION                              | 0.60                      |
| 2. DISTRIBUTION AND SALES                      | 0.60                      |
| 3. RESEARCH AND DEVELOPMENT                    | 0.30                      |
| 6. TOTAL COST OF PRODUCT, 4A + 5               | 11.56                     |

PLANT INVESTMENT (FIXED CAPITAL), 15.00 MILLION DOLLARS

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by product credit and general expenses (administration, distribution, etc.) charges which are required in solar cell grade silicon production by a specific process technology.

Application of the computer model to the Battelle process ( $\text{Zn/SiCl}_4$ ) indicated \$10,510,000 fixed capital investment and \$9.63/KG of silicon for a 1000 metric ton/yr. plant.

Work efforts were also initiated to standardize cost techniques utilized for economic analyses of the various alternate processes. This work is important to assure valid comparisons between processes. Initial base case conditions and utility cost information is summarized.

## V. PLANS

Plans for the next reporting period are summarized below:

### 1. Task 1.

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

Perform additional correlation activities on experimental data.

### 2. Task 2.

Continue technical interchange with Union Carbide as required on revised process flowsheet.

Continue work activity on preliminary process design for the conventional polysilicon process.

### 3. Task 3.

Continue work on cost standardization considerations for application to various alternate processes.

Perform additional development of computer model for plant investment and operating cost estimates.

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MILESTONE CHART

| TASK                        | 1975 |   |   | 1976 |   |   |   |   |   |   | 1977 |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
|-----------------------------|------|---|---|------|---|---|---|---|---|---|------|---|---|---|---|---|---|---|---|---|---|---|---|---|--|
|                             | O    | N | D | J    | F | M | A | M | J | J | A    | S | O | N | D | J | F | M | A | M | J | J | A | S |  |
| 1. Analyses of Process      |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| <u>System Properties</u>    |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 1. Prel. Data Collection    |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 2. Data Analysis            |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 3. Estimation Methods       |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 4. Exp.-Corr. Activities    |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 5. Prel. Prop. Values       |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 2. Chemical Engineering     |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| <u>Analyses</u>             |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 1. Prel. Process Flow Diag. |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 2. Reaction Chemistry       |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 3. Kinetic Rate Data        |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 4. Major Equip. Req.        |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 5. Chem. Equil.-Exp. Act.   |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 6. Process Comparison       |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 3. Economic Analyses        |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 1. Cap. Invest. Est.        |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 2. Raw Materials            |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 3. Utilities                |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 4. Direct Manuf. Costs      |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 5. Indirect Costs           |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 6. Total Cost               |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| 7. Process Comparison       |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |
| Final Report                |      |   |   |      |   |   |   |   |   |   |      |   |   |   |   |   |   |   |   |   |   |   |   |   |  |

- 1. Analyses of Process
  - System Properties
  - 1. Prel. Data Collection
  - 2. Data Analysis
  - 3. Estimation Methods
  - 4. Exp.-Corr. Activities
  - 5. Prel. Prop. Values
- 2. Chemical Engineering
  - Analyses
  - 1. Prel. Process Flow Diag.
  - 2. Reaction Chemistry
  - 3. Kinetic Rate Data
  - 4. Major Equip. Req.
  - 5. Chem. Equil.-Exp. Act.
  - 6. Process Comparison
- 3. Economic Analyses
  - 1. Cap. Invest. Est.
  - 2. Raw Materials
  - 3. Utilities
  - 4. Direct Manuf. Costs
  - 5. Indirect Costs
  - 6. Total Cost
  - 7. Process Comparison
- Final Report