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FINAL REPORT
Covering the Period October 1, 1975 - February 6, 1981
on

PROCESS FEASIBILITY STUDY IN SUPPORT OF SILICON MATERIAL TASK I

JPL Contract No. 954343

Silicon Material Task
Low-Cost Solar Array Project
to
JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
by

Carl L. Yaws
Ku-Yen Li
Jack R. Hopper
C. S. Fang
Keith C. Hansen

February 6, 1981

This work was performed for the Jet Propulsion Laboratory, California Institute of Technology, under NASA Contract NAS7100 for the U.S. Department of Energy, Division of Solar Energy.

The JPL Low-Cost Solar Array Project is funded by DOE and forms part of the DOE Photovoltaic Conversion Program to initiate a major effort toward the development of low-cost solar arrays.

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DISCLAIMER

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ABSTRACT

The Low-Cost Solar Array (LSA) Project at Jet Propulsion Laboratory (JPL) in Pasadena, California is being funded by the Department of Energy (DOE) for effective cost reduction in the production of silicon for solar cells. This study reports work performed at Lamar University in support of the LSA Project and presents results for process system properties, chemical engineering and economic analyses of the new technologies and processes being developed for the production of lower cost silicon for solar cells.

Analyses of process system properties are important for chemical materials involved in the several processes under consideration for semiconductor and solar cell grade silicon production. Major physical, thermodynamic and transport property data are reported for the following silicon source and processing chemical materials

- Silane
- Silicon Tetrachloride
- Trichlorosilane
- Dichlorosilane
- Silicon Tetrafluoride
- Silicon

The property data are reported for critical temperature, critical pressure, critical volume, vapor pressure, heat of vaporization, heat capacity, density, surface tension, viscosity, thermal conductivity, heat of formation and Gibb's free energy of formation. The reported property data are presented as a function of temperature to permit rapid usage in research, development and production engineering.

Chemical engineering analyses involving the preliminary process design of a plant (1000MT/yr capacity) to produce silicon via the technology under consideration were accomplished for the following processes:

- UCC Silane Process for Silicon
- BCL Process for Silicon - Case A
- BCL Process for Silicon - Case B
- Conventional Polysilicon Process (Siemens Technology)
- SiI_4 Decomposition Process
- DCS Process (Dichlorosilane)

Major activities in the chemical engineering analyses included base case conditions, reaction chemistry, process flowsheet, material balance, energy balance, property data, equipment design, major equipment list, production labor and forward for economic analysis. The process design package provided detailed

data for raw materials, utilities, major process equipment and production labor requirements necessary for polysilicon production in each process.

Using detailed data from the process design package, economic analyses for a 1000MT/yr silicon plant were accomplished for the processes under consideration for production of lower cost silicon. Primary results issuing from the economic analyses included plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

Cost and profitability results issuing from the chemical engineering and economic analyses are summarized below:

Process	Product Cost, $/kg (1980 dollars)	Sales Price, $/kg (1980 dollars)
•UCC Silane Process for Silicon	9.66	13.00 @ 15% DCF
•BCL Process for Silicon - Case A	12.08	13.28 @ 5% DCF
•BCL Process for Silicon - Case B	11.07	13.14 @ 10% DCF
•Conventional Polysilicon Process Siemens Technology)	53.77	--------------
•SiI_4 Decomposition Process	62.50	71.48 @ 5% DCF

For the summary tabulation, the product cost represents all cost associated with producing silicon including direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses. The sales price includes a profit for he company measured in terms of DCF (discounted cash flow) rate of return on the capital investment that the company spent in going into the business.

The cost and profitability analysis results of $9.66 and $13 per kg (1980 dollars) at 15% DCF for producing silicon by the UCC silane process (Union Carbide Corporation) indicate that this new technology for producing polysilicon shows good promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

For the BCL process - Cases A and B (Battelle Columbus Laboratories), cost and profitability results are $11.07 - 12.08 and $13.14 - 13.28 per kg (1980 dollars) at 5 - 10% DCF rate of return. These results indicate that this new technology for producing polysilicon shows promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

For the conventional polysilicon process, the cost analysis is based on a poly plant constructed in the 1960's (1965 or earlier) since several existing plants producing semiconductor grade polysilicon in the United States were constructed in the 1960's. The operating costs for the plant are applicable to the time period of interest such as 1980. The average product cost, $53.77 per kg (1980 dollars), for the conventional polysilicon process corresponds to intermediate electrical costs (3.15 ¢/kw hr for 1980). These costs results for the conventional polysilicon process indicate that this Siemens technology using trichlorosilane for producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

The cost and profitability results of $62.5 and $71.48 per kg (1980 dollars) at 5% DCF rate of return for the SiI_4 decomposition process indicate that this new technology for producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

Using a hot wire method, gas phase thermal conductivity values of argon, hydrogen, silane, dichlorosilane, trichlorosilane, tetrachlorosilane and tetrafluorosilane were experimentally determined between 25°C and 350°C. Comparison of the values obtained in the study for argon and hydrogen with previously reported values indicated that the values should be accurate to ±2% throughout the temperature range.

Using a transpiration technique, gaseous viscosity values for nitrogen, dichlorosilane, trichlorosilane, and tetrafluorosilane were experimentally determined between 40°C and 200°C. Comparison of the values obtained in the study for nitrogen with previously reported viscosity values indicate that the values obtained are accurate to ±2% throughout the temperature range

Studies were conducted to develop a method of generating silicon tetrafluoride from hexafluorasilicic acid, a readily available by-product of the phosphate fertilizer industry. Conditions for the efficient precipitation of two SiF_4 precursors (Na_2SiF_6 and $BaSiF_6$) were determined. These precursors were then thermally decomposed to generate SiF_4. Parameters such as temperature, heating time, and flow rate necessary for efficient production of SiF_4 were determined.

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1. INTRODUCTION - BACKGROUND

The Low-Cost Solar Array Project (LSA) of Jet Propulsion Laboratory (JPL) had its beginning in 1975, and was concerned with achieving our national solar energy goal (1) to "develop at the earliest feasible time those applications of solar energy that can be made economically attractive and environmentally acceptable as alternate energy sources." Solar cell grade silicon for photovoltaic systems will need to be produced in great volume at considerable reduced prices to accomplish this significant energy goal.

The Low-Cost Solar Array (LSA) Project at Jet Propulsion Laboratory (JPL) in Pasadena, California is being funded by the Department of Energy (DOE) for effective cost reduction in the production of silicon for solar cells. An important overall objective of the project is to reduce the cost of electricity produced with solar cells from today's \$10-25 per W (Peak) to \$0.70 per W (1980 dollars) by 1986. Cost reductions for solar cells are allocated to major tasks encompassing everything from initial silicon production to final array assembly. The cost goal for the silicon material that goes into solar cells is about \$14 per kg of material (1980 dollars).

Semiconductor grade silicon which is currently produced via the conventional Siemens process by several major manufacturers (Dow-Corning, Monsanto, Motorola, Texas Instruments and Great Western) in the United States is too expensive to meet the silicon material cost goal. Lower cost silicon is needed for solar cells. Alternate processes that depart from the conventional process need to be developed by several concerns to produce a less costly silicon material.

Process evaluation - which is a very useful tool in research and development - is useful in investigation of such alternate processes for solar cell grade silicon. The planning and implementation of a research and development program involves decision making on what work can be left out with least jeopardy to short and long term consequences and what work should be pursued with the best chance for success in achieving short and long term goals. Early process evaluation investigation including preliminary economic evaluation aids the decision making involved in whether to commit extra funds to carry-out a project from research to large scale plant.

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1. ERDA, National Solar Energy Program, Industrial Briefing, NASA/JPL Low-Cost Silicon Solar Array Project, NASA Headquarters, Washington, D.C. (February 5, 1975).

The early study particularly minimizes the risks involved in the process development from early research to large scale plant. The process evaluation investigation should be initiated with the very inception of the research project and continued throughout its life until the project is proved successful or abandoned because it cannot effectively meet the financial and product purity goals.

In research and development, a screening out is required for those projects and processes which are believed to be unsound or least attractive. Economics dictate that the money should not be wasted on projects which may turn out to be useless. The many alternate projects and processes which are available necessitate the effective use of a screening procedure, not to locate a foolproof venture, but to try to select the best possible project.

Process evaluation investigation may effectively deal with a complete process or part of a process. Major cost areas of a process and profitability potential of a proposed process may be pinpointed. It is also equally valuable in comparing alternate processes and in the selection of processes with the best technical and economic features.

A typical sequence for process selection is presented in Figure 1-1.The process evaluation activities are shown in relation to their usefulness in the selection of a process for scale-up to pilot plant and large scale plant. These process evaluation activities (system properties, chemical engineering and economic analysis tasks) may be effectively utilized in the investigation of alternate processes for low cost, high volume production of silicon suitable for solar cells.

In this process feasibility study in support of Silicon Material Task I of the LSA, the proposed scope of work is to perform investigations and analyses of processes for the low cost, high volume production of silicon suitable for solar cells. The objective of this program is to validate the commercial practicality of these alternate processes based on the following process evaluation criteria:

1. Analyses of Process-System Properties
2. Chemical Engineering Analyses
3. Economic Analyses

Each of these evaluation criteria is focused on the production of solar cell grade silicon at greatly reduced cost.

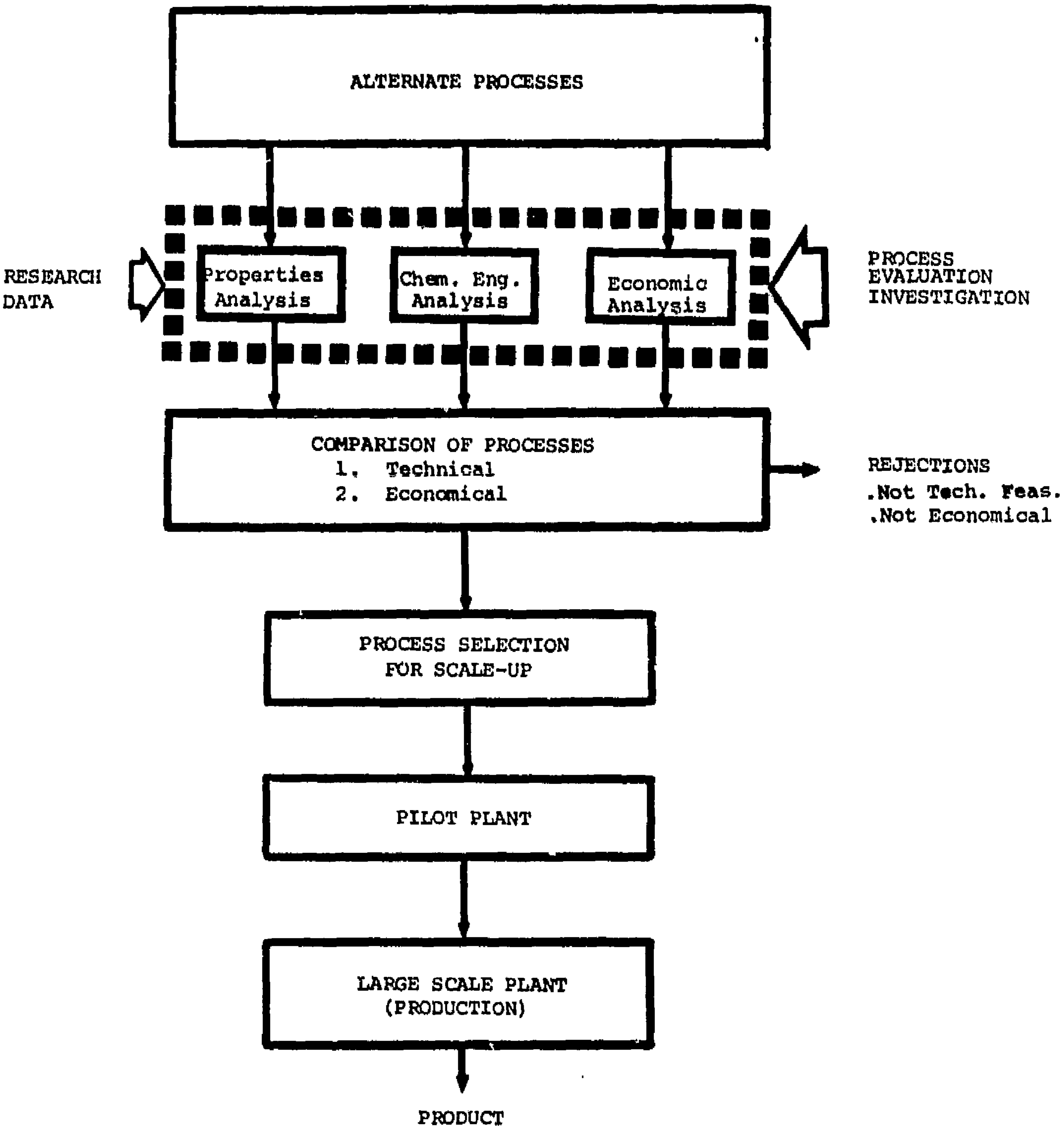

Figure 1-1 TYPICAL SEQUENCE FOR PROCESS SELECTION

2. PROCESS SYSTEM PROPERTIES ANALYSES

2.1 Silane Properties

Critical Properties (Table 2.1-1)

Experimental data for the critical temperature and pressure of silane are available (2, 15, 20, 22, 25, 27, 29, 45, 47, 49 50, 51). However, all sources cite Adwentowski (51), who prepared his sample from Mg_2Si and used the fraction boiling at -116°C. Since the boiling point of silane is generally accepted as -112°C, these data may not be completely reliable.

The critical compressibility factor, Z_c, was estimated by the Garcia-Barcena method:

$$Z_c = f(T_b) - g(T_b/M) \qquad (2.1\text{-}1)$$

where T_b = boiling point, °K; and M = molecular weight g/g - mol. The terms f (T_b) and g (T_b/M) are shown as a nomograph (29). Reid and Sherwood tested this equation using sixteen inorganic compounds and found an average deviation of 1.8%. The accuracy of the correlation was tested by applying it to similar inorganic and organic compounds (NH_3, N_2H_4, B_2H_6, CH_4). Average deviation was 3.6% for the compounds tested.

The critical volume was found by the real gas relation:

$$V_c = Z_c R T_c / P_c \qquad (2.1\text{-}2)$$

using the Adwentowski data and the estimated value of Z_c.

Vapor Pressure (Figure 2.1-1)

Observed vapor pressure data for silane are available (2, 13, 15, 18, 20, 25, 27, 36, 45, 51, 60) over nearly the entire liquid phase from melting point (mp) to boiling point (bp) to critical point (cp). The available data were correlated with the least squares technique for vapor pressure as a function of temperature using the following correlation relation (64):

$$\log P_v = A + \frac{B}{T} + C \log T + DT + ET^2 \qquad (2.1\text{-}3)$$

Average deviations were less than 3.5%. Greater deviations were encountered with other vapor pressure equations. For example, average absolute deviations exceeded 38% for the Cox-Antoine type equation.

Heat of Vaporization (Figure 2.1-2)

Heat of vaporization data for silane are available only at the boiling point (2, 21, 22, 23, 27, 41).

These data vary less than 1%. Watson's correlation (27, 29) was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_v = \Delta H_{v1}\left(\frac{T_c - T}{T_c - T_1}\right)^n \qquad (2.1\text{-}4)$$

where ΔH_{v1} is the heat of vaporization at the boiling point (T_1) and n = 0.38.

Heat Capacity (Figures 2.1-3 and 2.1-4)

Heat capacity of the ideal gas at atmospheric pressure is primarily based on structural and spectral data. Values from the various sources (5, 16, 20, 22, 25, 39, 44, 52) are in excellent agreement with differences less than 1%.

Liquid heat capacity data (6) 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 × density = constant. The constant value was .2895. Testing of the relationship with the available data produced average deviation of 7%.

Density (Figure 2.1-5)

Liquid density data for silane are available (2, 15, 18, 23, 25, 35, 48, 52) from the melting point to the boiling point. The Yaws-Shah equation (62) for density of the saturated liquid was used to extend the data to the critical point:

$$\rho = AB^{-(1-T_r)^{2/7}} \qquad (2.1\text{-}5)$$

where ρ = density, g/cm^3, 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 and experimental data was 1.48%.

Surface Tension (Figure 2.1-6,

Data for surface tension (7) are available from the melting point to the boiling point. These data were extended using the Othmer relation (29):

$$\sigma = \sigma_1\left(\frac{T_c - T}{T_c - T_1}\right)^n \qquad (2.1\text{-}6)$$

where σ_1 = surface tension at T_1, dynes/cm; T_c = critical emperature, °K; T = temperature, °K; and n = the correlation parameter, 1.2. Deviations between data and correlated values were less than 1%.

Viscosity (Figures 2.1-7 and 2.1-8)

The Stiel and Thodos correlation (29) was used to augment limited data on gas viscosity (2, 15, 20, 23, 25, 52, 53, 57) at atmospheric pressure. All data sources cite Rankine (57) who made his measurement in 1922 at 15° and 100°C. Deviations between data and correlation were less than 1% for the two data values.

Liquid viscosity data are available (30) in the temperature range between the melting point and boiling point. The data were extended to cover the entire liquid range with the following correlation (63) for viscosity of the saturated liquid as a function of temperature:

$$\log \mu_L = A + B/T + CT + DT^2 \qquad (2.1\text{-}7)$$

Correlation values and data were in good agreement with average absolute deviation of 1.4%.

Thermal Conductivity (Figures 2.1-9 and 2.1-10)

Gas thermal conductivity for silane was estimated by the modified Eucken correlation for polyatomic gases. The Eucken correlation agrees well with Svehla (40); deviations were less than 1%. There are no experimental data available for gas thermal conductivity.

Liquid thermal conductivity for silane was estimated with the modified Stiel and Thodos relation (29). The correlation was tested with experimental data for methane. The average deviations were less than 17%. The deviations for silane are probably in the same range. The presented results are intended to represent correct order-of-magnitude values.

Heat of Formation and Free Energy of Formation (Figures 2.1-11 and 2.1-12)

Values for the heat of formation, ΔH_f, and free energy of formation, ΔG_f, are available from American (39) and Russian (12) sources. Average values were selected. The deviation between data and selected results was 0.2 K cal/mol.

TABLE 2.1-1--CRITICAL CONSTANTS AND PHYSICAL PROPERTIES OF SILANE

Identification	Silane
Formula	SiH_4
State (std. cond.)	gas (colorless)
Molecular Weight, M	32.12
Boiling Point, T_b, °C	-111.9
Melting Point, T_m, °C	-184.7
Critical Temp, T_c, °C	-3.5 (Questionable Value)
Critical Pressure, P_c, atm	47.8 (Questionable Value)
Critical Volume, V_c, cm^3/gr mol	130.06 (Estimated)
Critical Compressibility Factor, Z_c	0.281 (Estimated)
Critical Density, ρ_c gr/cm^3	0.247 (Estimated)
Acentric Factor (Ω)	0.0774

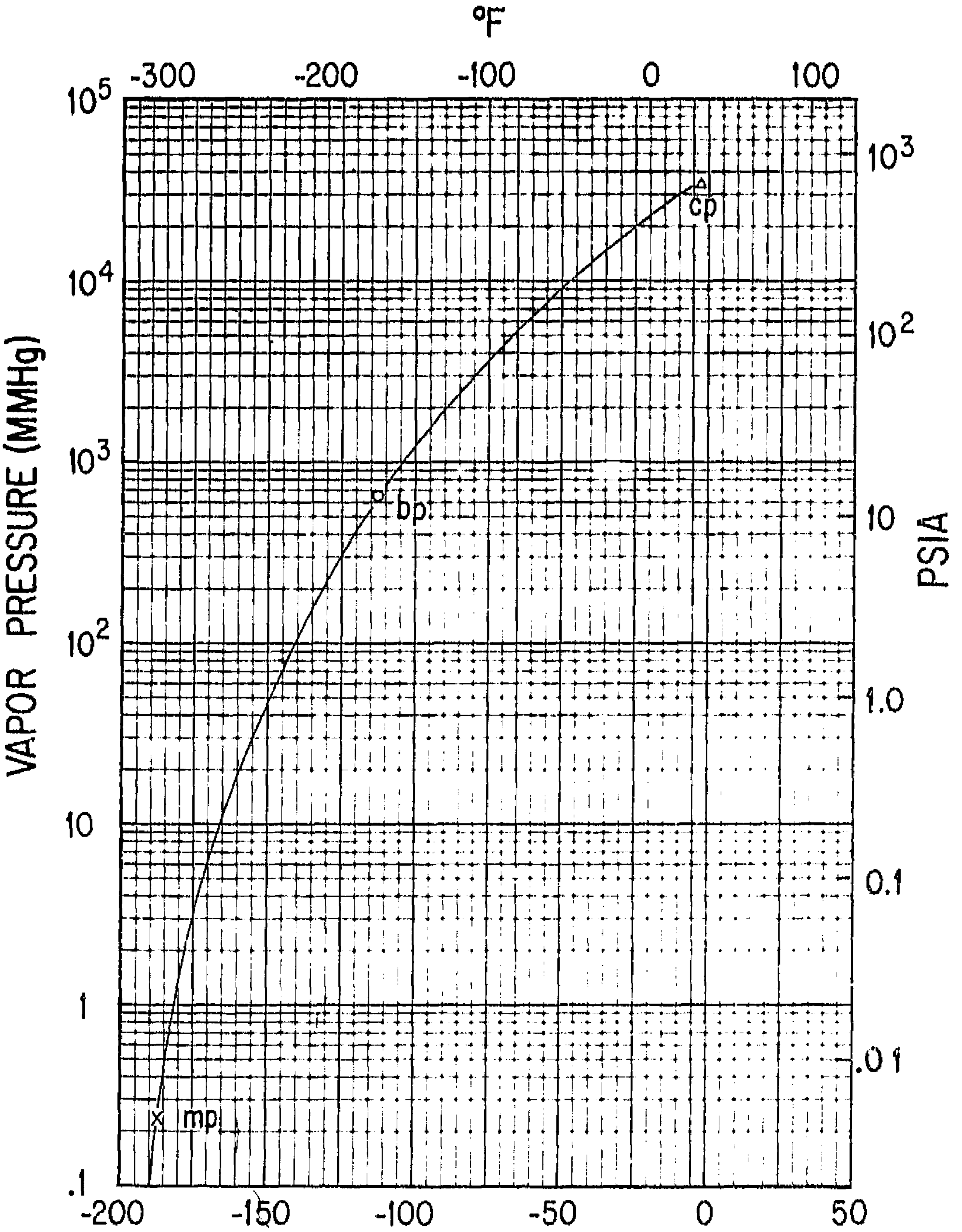

Figure 2.1-1 Vapor Pressure vs. Temperature for Silane

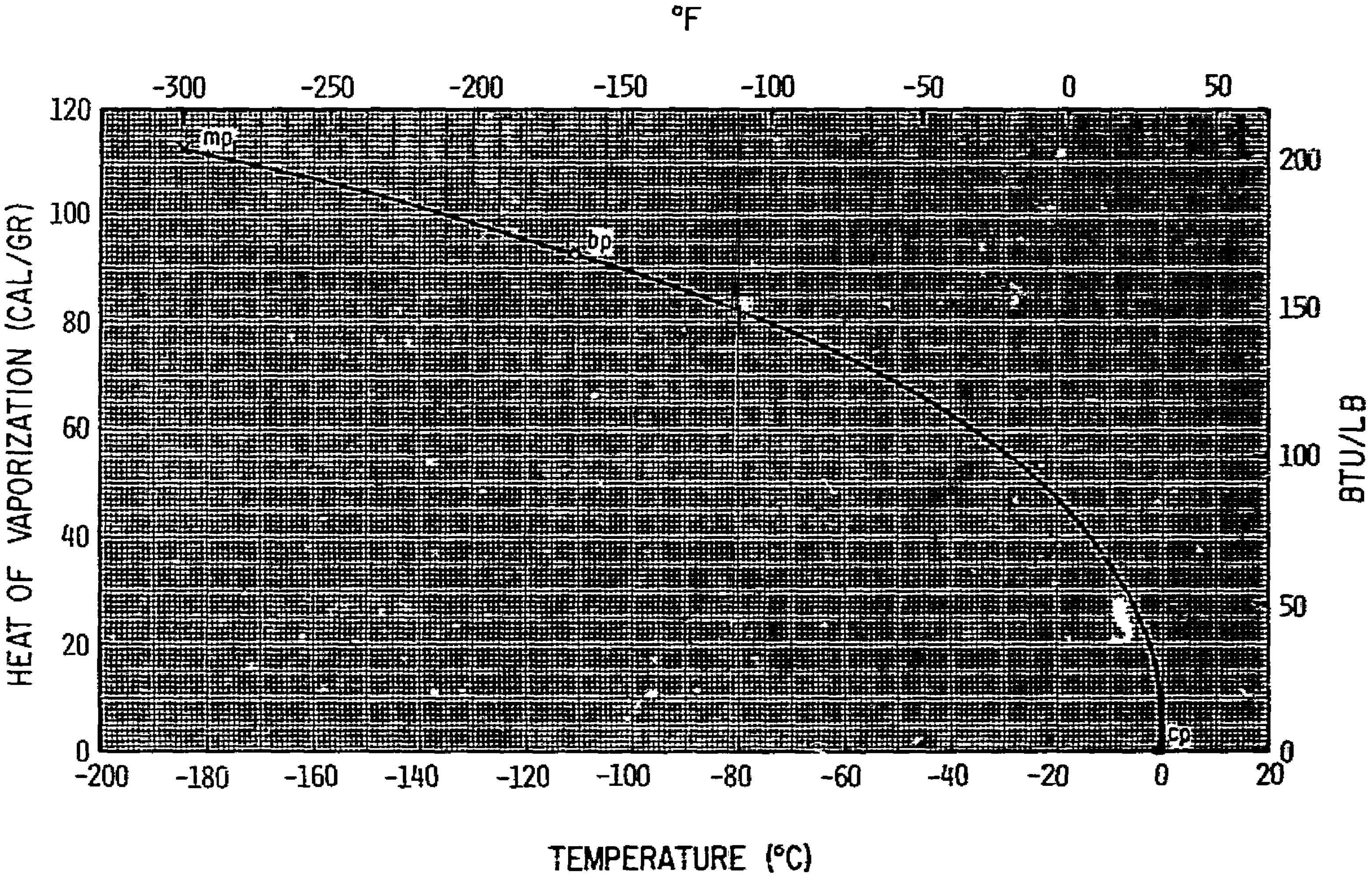

Figure 2.1-2 Heat of Vaporization vs. Temperature for Silane

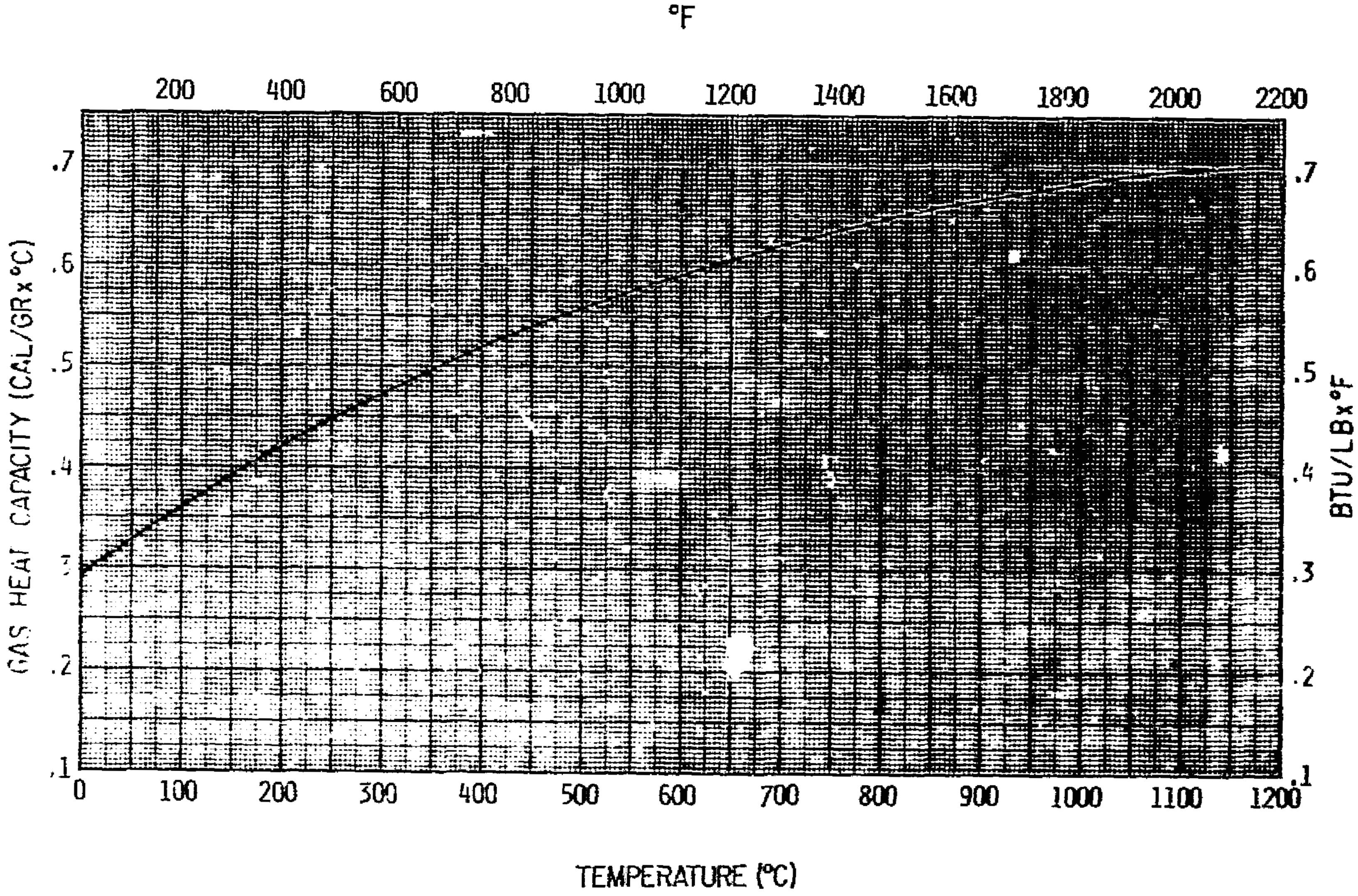

Figure 2.1-3 Gas Heat Capacity vs. Temperature for Silane

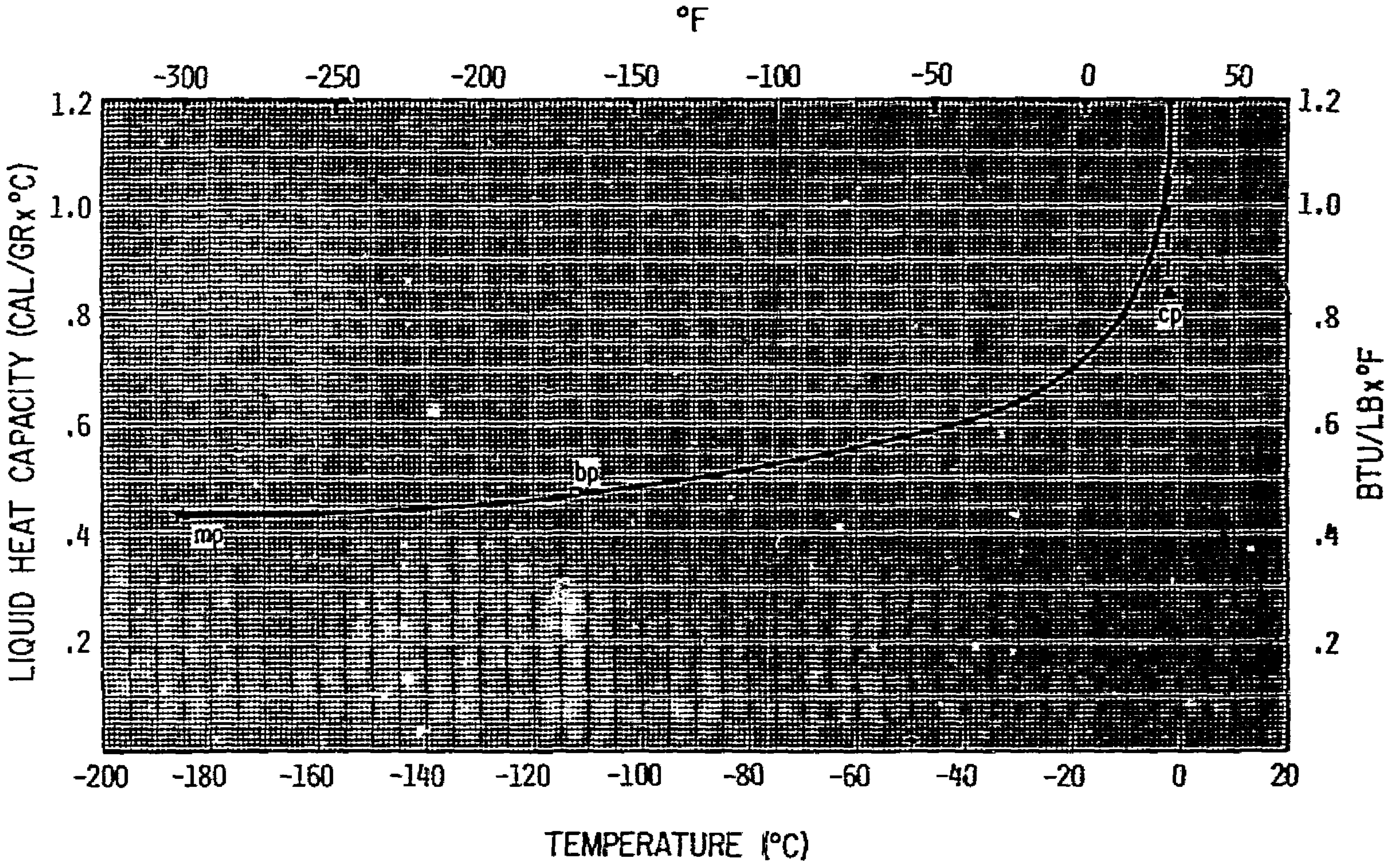

Figure 2.1-4 Liquid Heat Capacity vs. Temperature for Silane

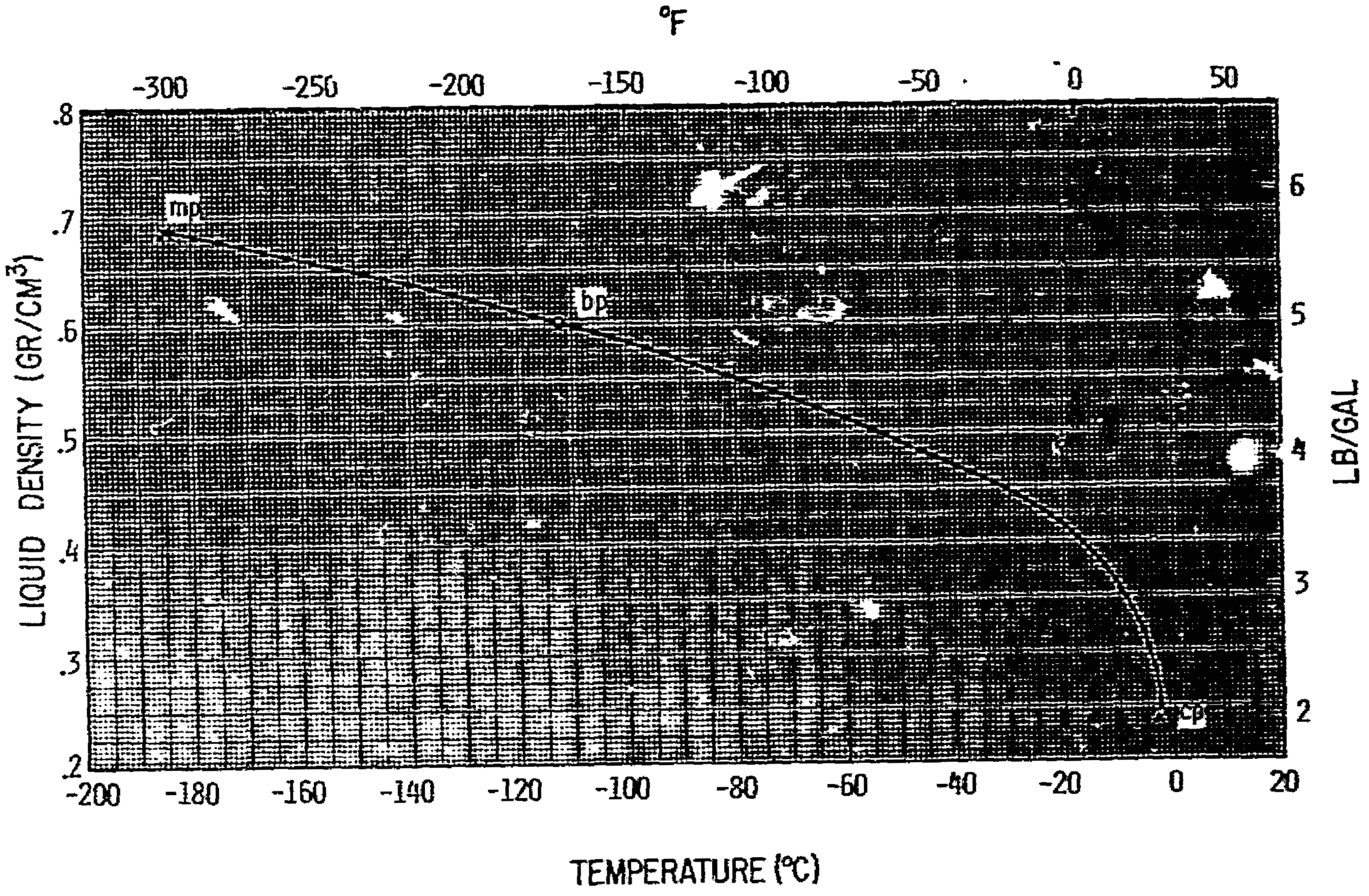

Figure 2.1-5 Liquid Density vs. Temperature for Silane

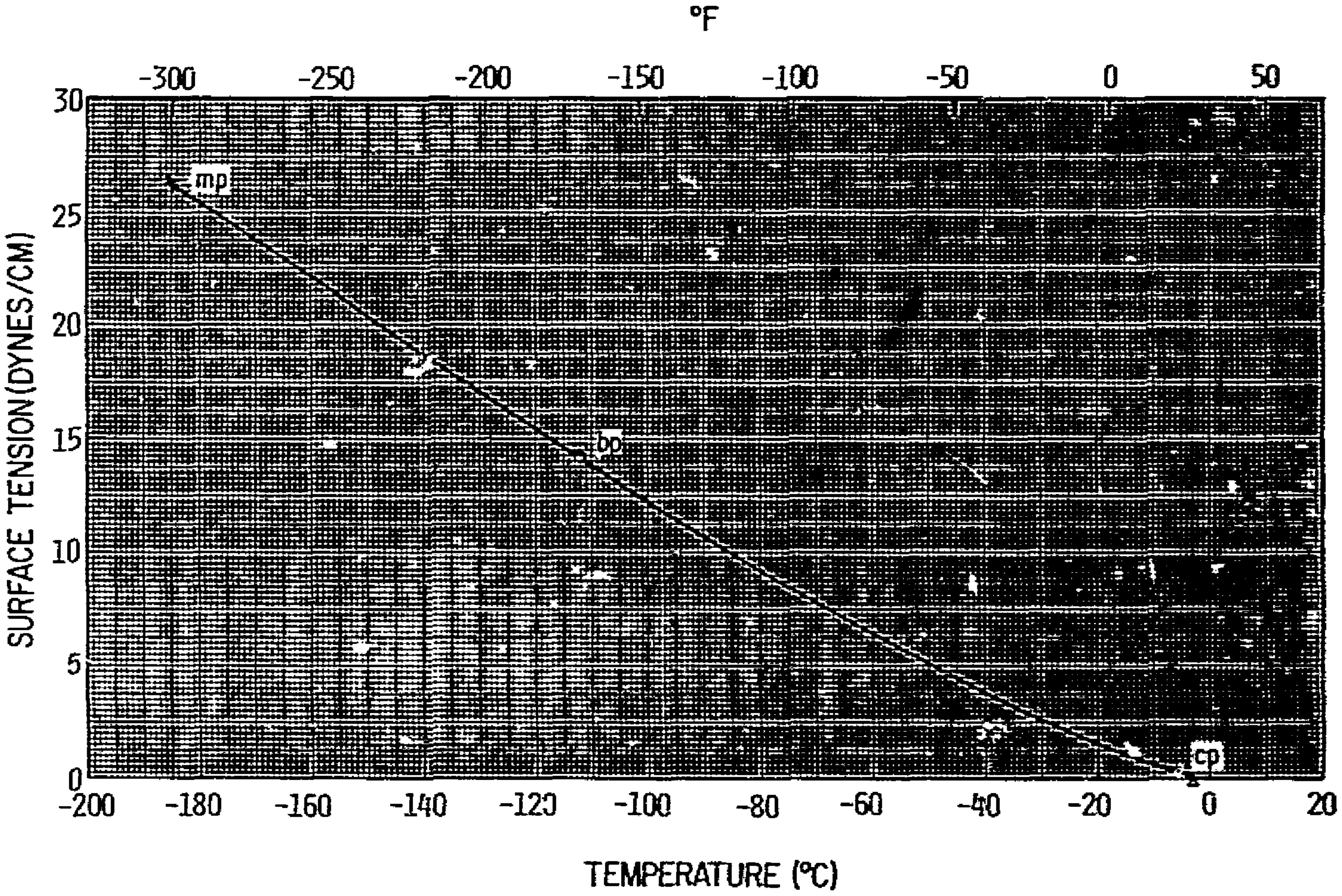

Figure 2.1-6 Surface Tension vs. Temperature for Silane

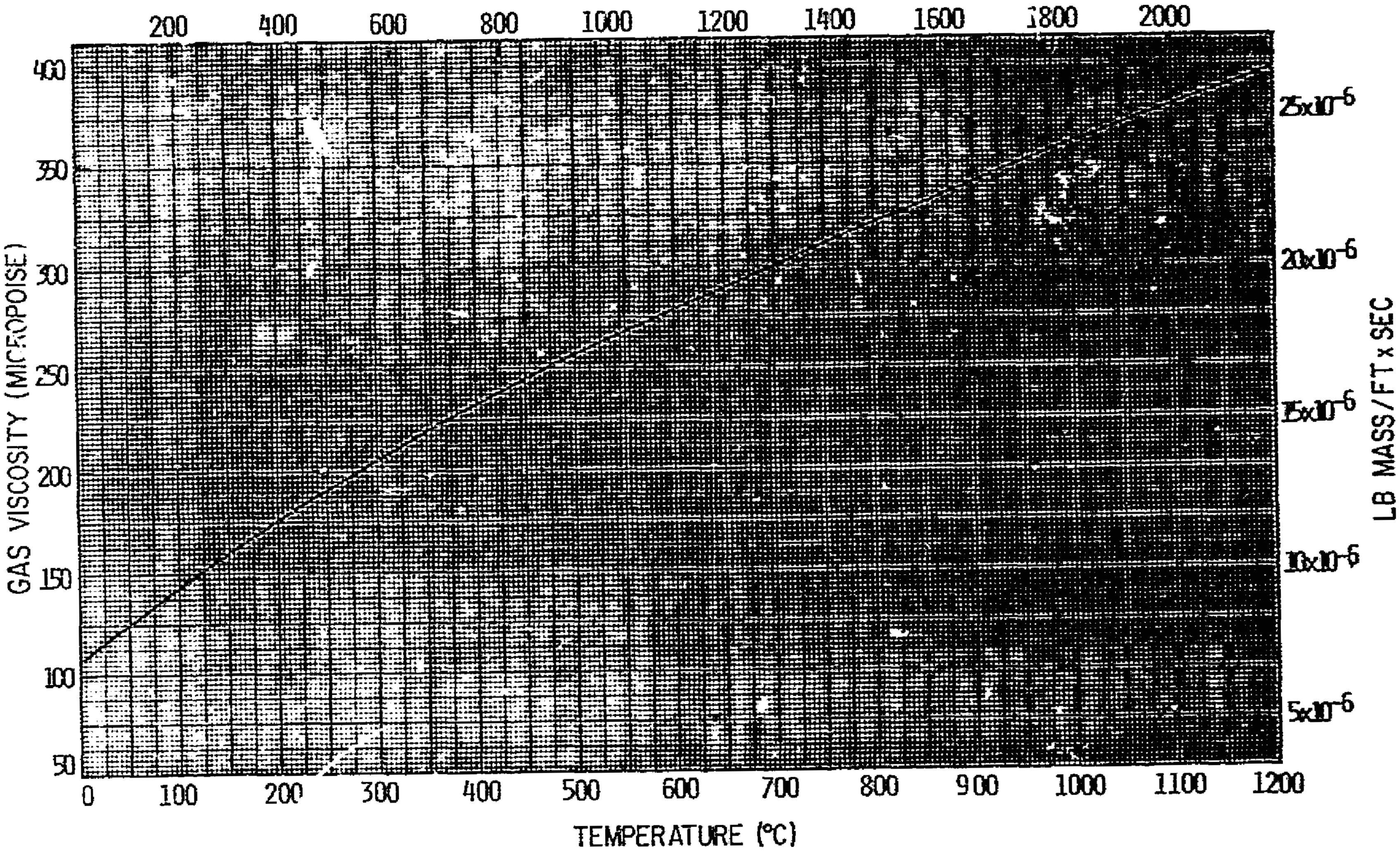

Figure 2.1-7 Gas Viscosity vs. Temperature for Silane

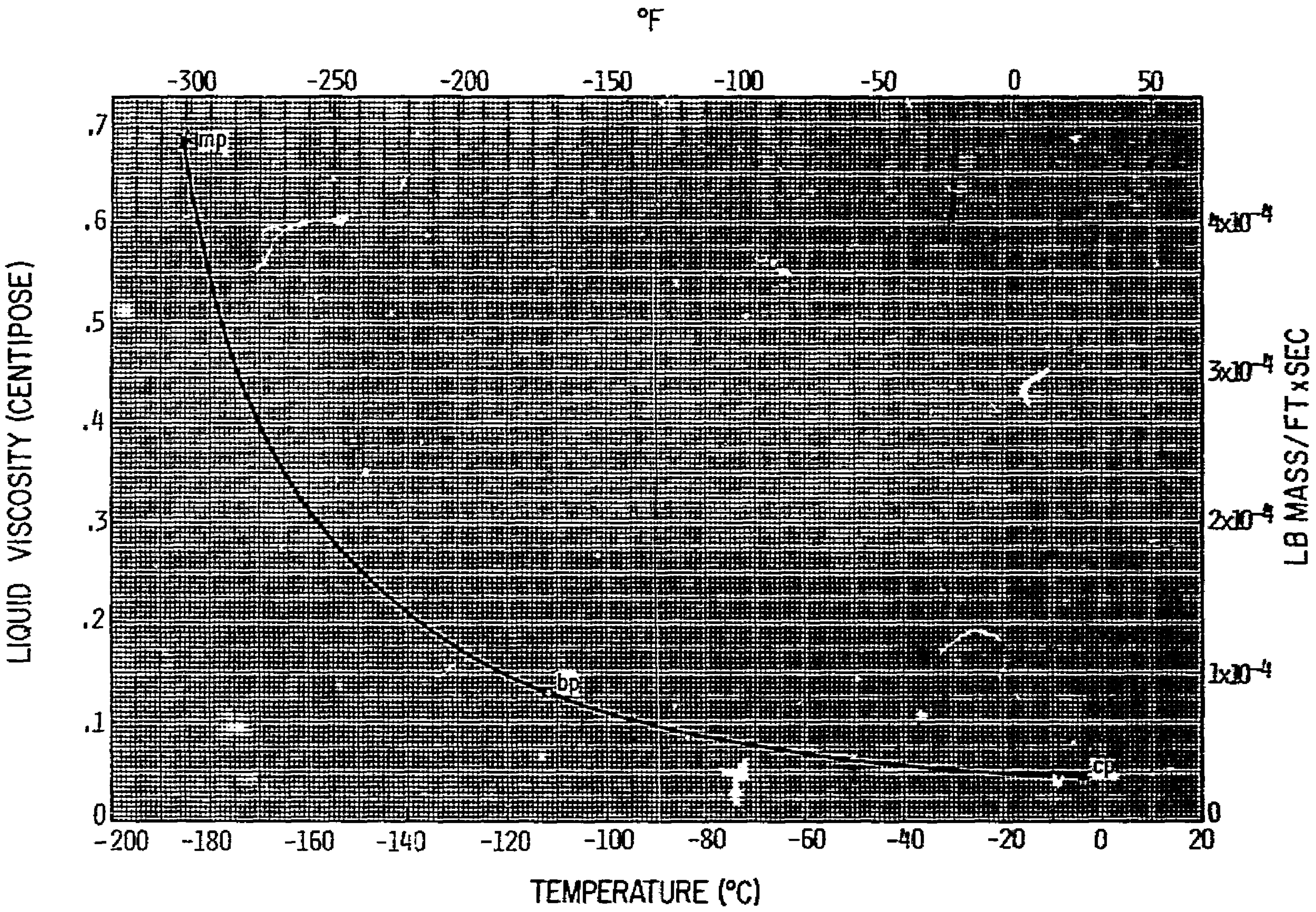

Figure 2.1-8 Liquid Viscosity vs. Temperature for Silane

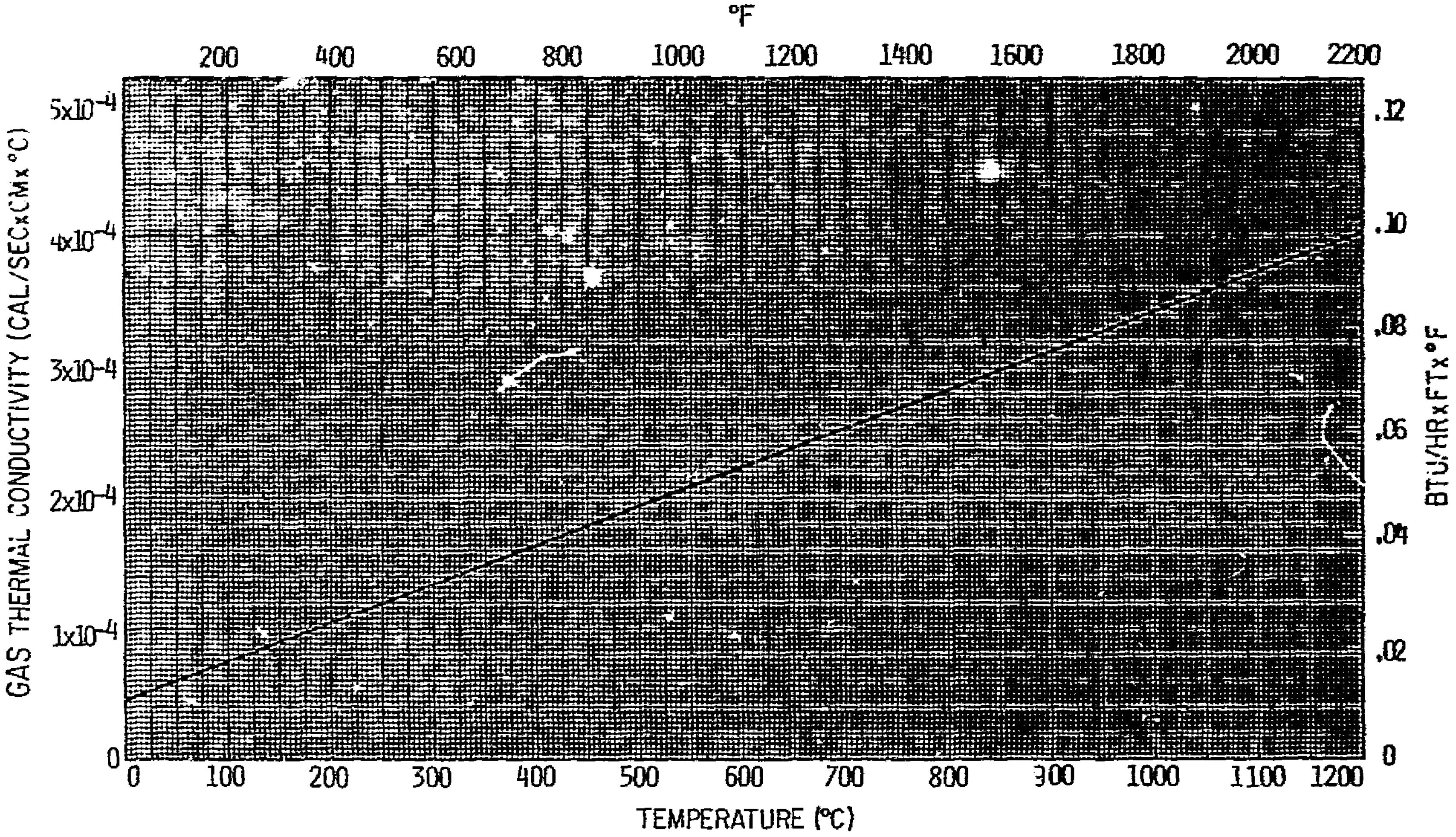

Figure 2.1-9 Gas Thermal Conductivity vs. Temperature for Silane

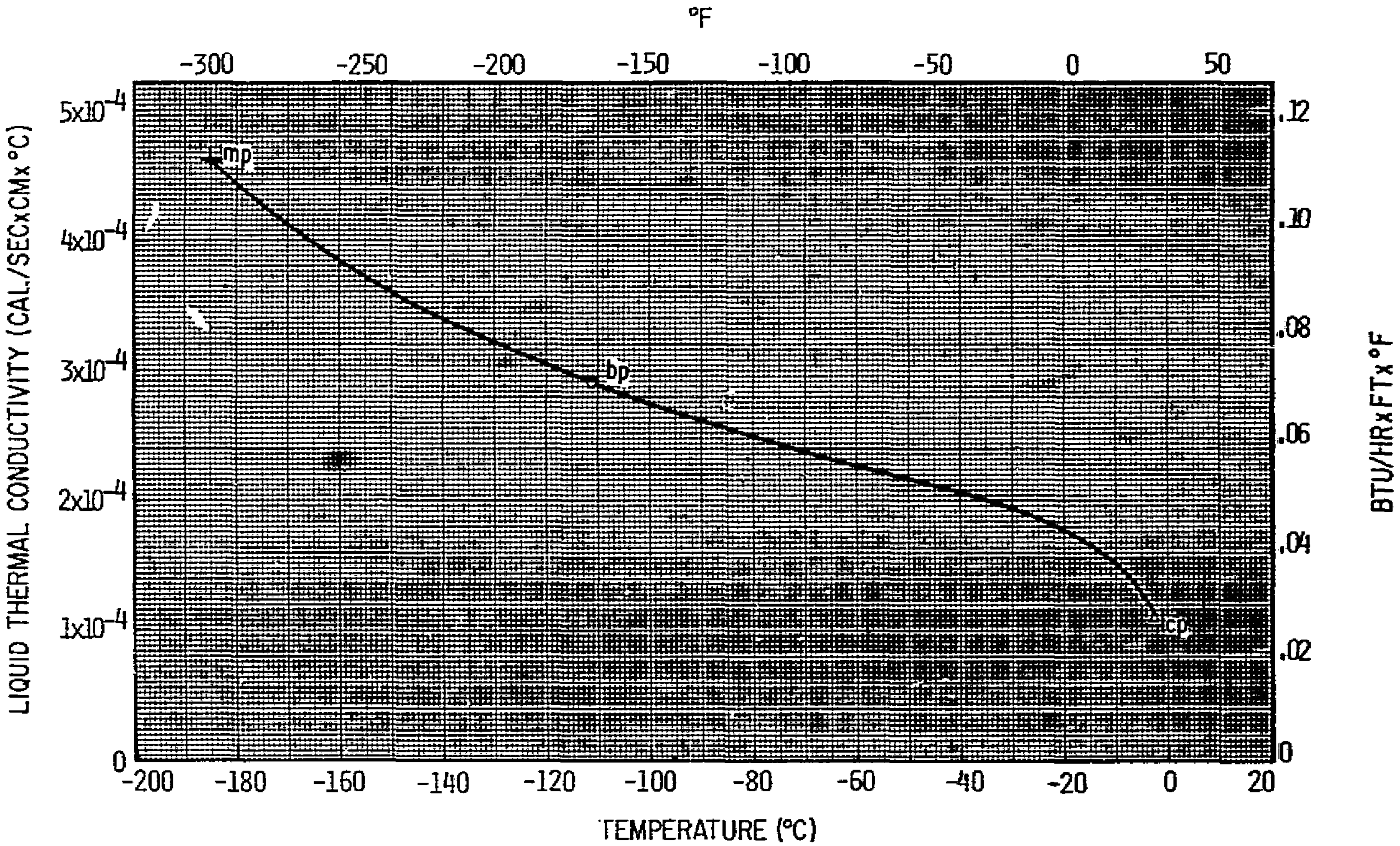

Figure 2.1-10 Liquid Thermal Conductivity vs. Temperature for Silane

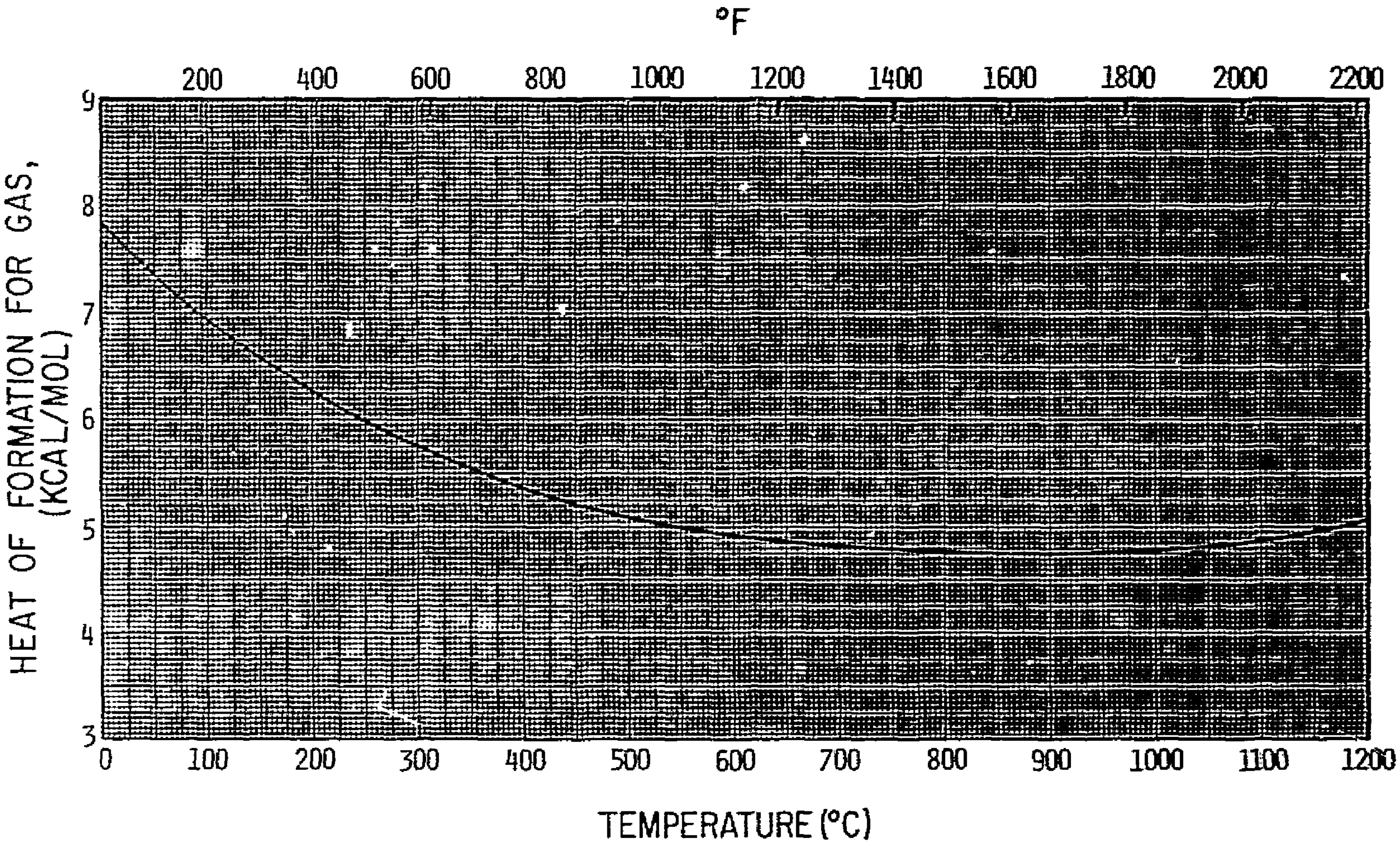

Figure 2.1-11 Heat of Formation vs. Temperature for Silane

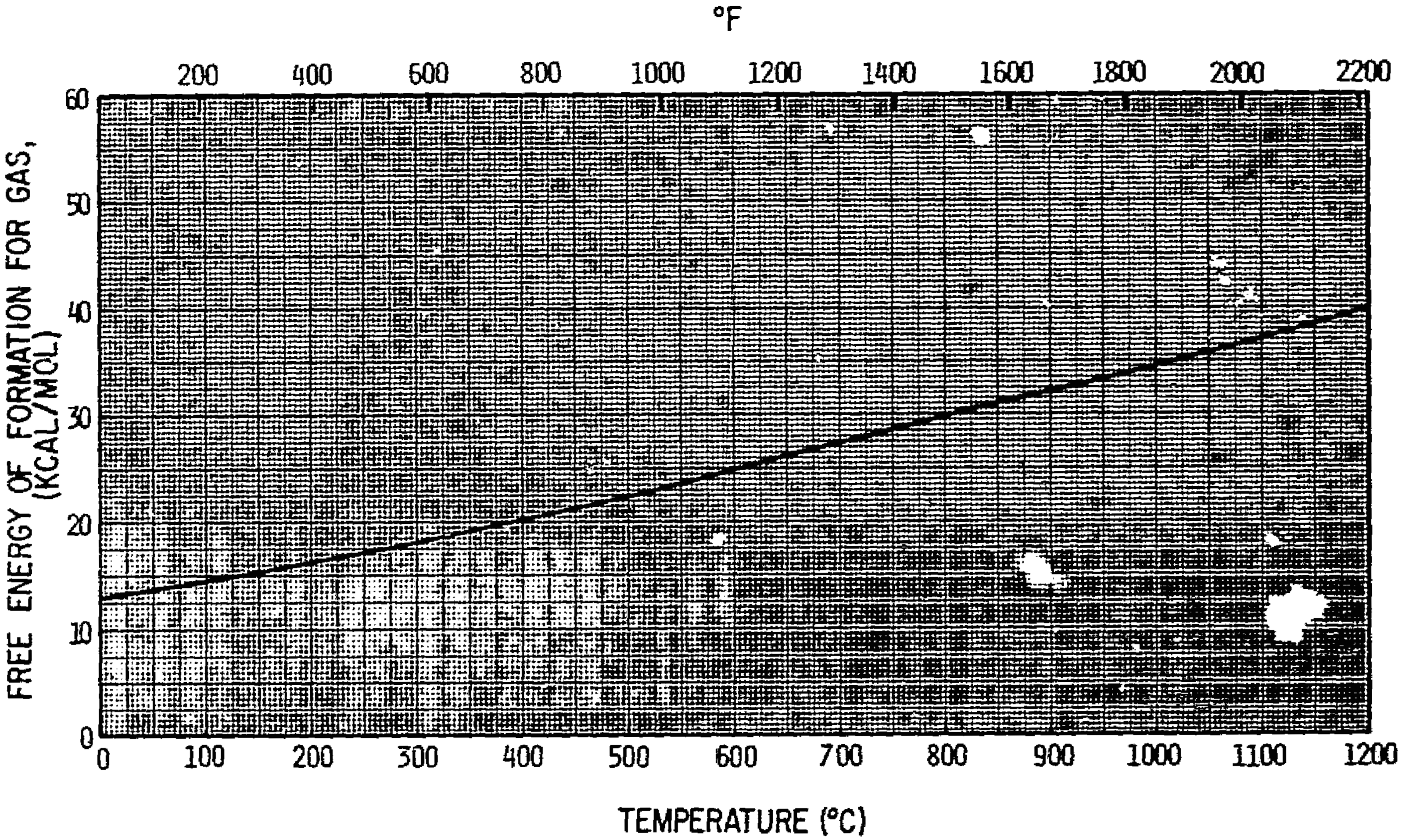

Figure 2.1-12 Free Energy of Formation vs. Temperature for Silane

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2.2 Silicon Tetrachloride Properties

Critical Properties (Table 2.2-1)

Experimental results for the critical temperature, pressure and volume of silicon tetrachloride are available (B5, B8, B9, B11, B32, B33, B35, B36, B44, B50, B56, B59, B82, B83). The results among the several investigators are in general agreement. Deviations from the selected values are 1.71%, 0.5%, and 10.8% respectively for critical temperature, pressure and volume.

The critical compressibility factor, Z_c, was calculated using the following equation:

$$Z_c = P_cV_c/RT_c \qquad (2.2\text{-}1)$$

Also given in the table are values for the acentric factor, ω which is defined by:

$$\omega = -\log P_r - 1.000 \text{ (at } T_r = 0.70) \qquad (2.2\text{-}2)$$

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

Vapor Pressure (Figure 2.2-1)

Experimental vapor pressure data for silicon tetrachloride are available (B7, B22, B24, B27, B30, B32, B43, B53, B78, B103) from slightly above the melting point (mp) to boiling point (bp) and at the critical point (cp). Available data were extrapolated using the YSSP vapor pressure correlation (B102):

$$\log P_v = A + \frac{B}{T} + C \log T + DT + ET^2 \qquad (2.2\text{-}3)$$

where

P_v = vapor pressure of saturated liquid, mm of Hg

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

T = temperature, °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.

Heat of Vaporization (Figure 2.2-2)

Heat of vaporization data for silicon tetrachloride are available only at the boiling point (B5, B11, B22, B30, B36, B65, B82, B86). Watson's correlation was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_v = \Delta H_{v_1} \left[\frac{T_c - T}{T_c - T_1}\right]^n \qquad (2.2\text{-}4)$$

where ΔH_{v_1} is the heat of vaporization at the boiling point (T_1) and $n = 0.38$.

Heat Capacity (Figures 2.2-3 and 2.2-4)

Heat capacity data for silicon tetrachloride as ideal gas at low pressure are available (B3, B10, B17, B20, B28, B32, B34, B43, B45, B52, B67, B73, B76, B82, B84, B86, B91). The values, which are primarily based on structural and spectral measurements, are in close agreement.

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

$$C_p = A + BT + CT^2 + DT^3 \qquad (2.2\text{-}5)$$

where C_p - heat capacity of ideal gas at low pressure, cal/(g-mol)(°K); A, B, C and D = characteristic constants for the chemical compounds; and T = temperature, °K. Average absolute deviation is about 0.6%.

Liquid heat capacity data are available (B5, B22, B28, B30, B26, B43, B52, B60, B65, B76, B77, B82, B104) in the mp-bp temperature interval. The data were extended to cover the entire liquid phase with the relation:

$$\text{liquid heat capacity} \times \text{density} = \text{constant} \qquad (2.2\text{-}6)$$

The constant value was 0.3054. Testing of the relationship with the available data produced average deviation of 4%.

Density (Figure 2.2-5)

Liquid density data are available (B1, B49, B50, B59, B65, B77, B79, B81, B82) from near the melting point to the critical point. The Yaws-Shah equation (B100, B107) for denisty of the saturated liquid was used to extend the data to the critical point:

$$\rho = AB^{-(1-T_r)^{2/7}} \qquad (2.2\text{-}7)$$

The agreement of calculated and experimental values was very good with average absolute deviation of only 0.44%.

Surface Tension (Figure 2.2-6)

Data for surface tension (B5, B22, B27, B49, B82) are available in the melting point to boiling point temperature range. The data were extended using the Othmer realtion:

$$\sigma = \sigma_1 \left[\frac{T_c - T}{T_c - T_1} \right]^n \qquad (2.2\text{-}8)$$

where σ_1 = surface tension at T_1, dynes/cm

T_c = critical temperature, °K

T = temperature, °K

and n = the correlation parameter, 1.14. Testing of the relationship with the available data produced average deviation of less than 1%.

Viscosity (Figure 2.2-7 and 2.2-8)

The modified Yoon and Thodos correlation (B105, B106) was used to augment limited data (B36, B51) on gas viscosity at low pressure:

$$\eta\xi = 4.610\ T_r^{0.618} - 2.04\ e^{-0.449\ T_r} + 1.94\ e^{-4.058\ T_r} + 0.1 \qquad (2.2\text{-}9)$$

where $\xi = T_c^{1/6} M^{-1/2} P_c^{-2/3}$

The deviation between data and correlation was 2%.

Liquid viscosity data are available (B5, B8, B32, B36, B49, B51, B107) in both mp-bp and bp-cp temperature ranges. The data were extended to cover the entire liquid range with the following correlation (B107) for viscosity of the saturated liquid as a function of temperature.

$$\log \mu_L = A + B/T + CT + DT^2 \qquad (2.2\text{-}10)$$

Average deviation between correlation and data was less than 3%.

Thermal Conductivity (Figure 2.2-9 and 2.2-10)

Gas-phase thermal conductivity data are available (B75, B109) in the temperature range of 70 to 300°C. The data were correlated by a series expansion in temperature (B107):

$$\lambda_G = A + BT + CT^2 + DT^3 \qquad (2.2-11)$$

where λ_G = gas thermal conductivity, cal/cmxsecx°C; A, B, C and D = characteristic constants for the chemical compounds and T = temperature, °K. The extimates of Svehla (B73) agree with the above correlation. The deviation between data and correlation values was 1.10%.

Thermal conductivity for liquid phase is available (B25) at only one temperature (32°C). The modified Stiel and Thodos equation (B107) was used to cover the entire saturated-liquid phase.

Heat and Free Energy of Formation (Figures 2.2-11 and 2.2-12)

Values for the heat of formation (ΔH_f) and Gibbs' free energy of formation (ΔG_f) for the ideal gas are available from American (B72) and Russian (B17, B64) sources. American values were selected.

TABLE 2.2-1

CRITICAL CONSTANTS AND PHYSICAL PROPERTIES OF SILICON TETRACHLORIDE

Identification	Silicon Tetrachloride
Formula	$SiCl_4$
State (Std. Cond.)	Liquid
Molecular Weight, M	169.90
Boiling Point, T_b, °C	57.3
Melting Point, T_m, °C	-69.4
Critical Temp., T_c, °C	234.0
Critical Pressure, P_c, atm	37.0
Critical Volume, V_c, cm^3/grmol	326.3
Critical Compressibility Factor, Z_c	0.290
Critical Density, ρ_c, gr/cm^3	0.5207
Acentric Factor, ω	0.2556

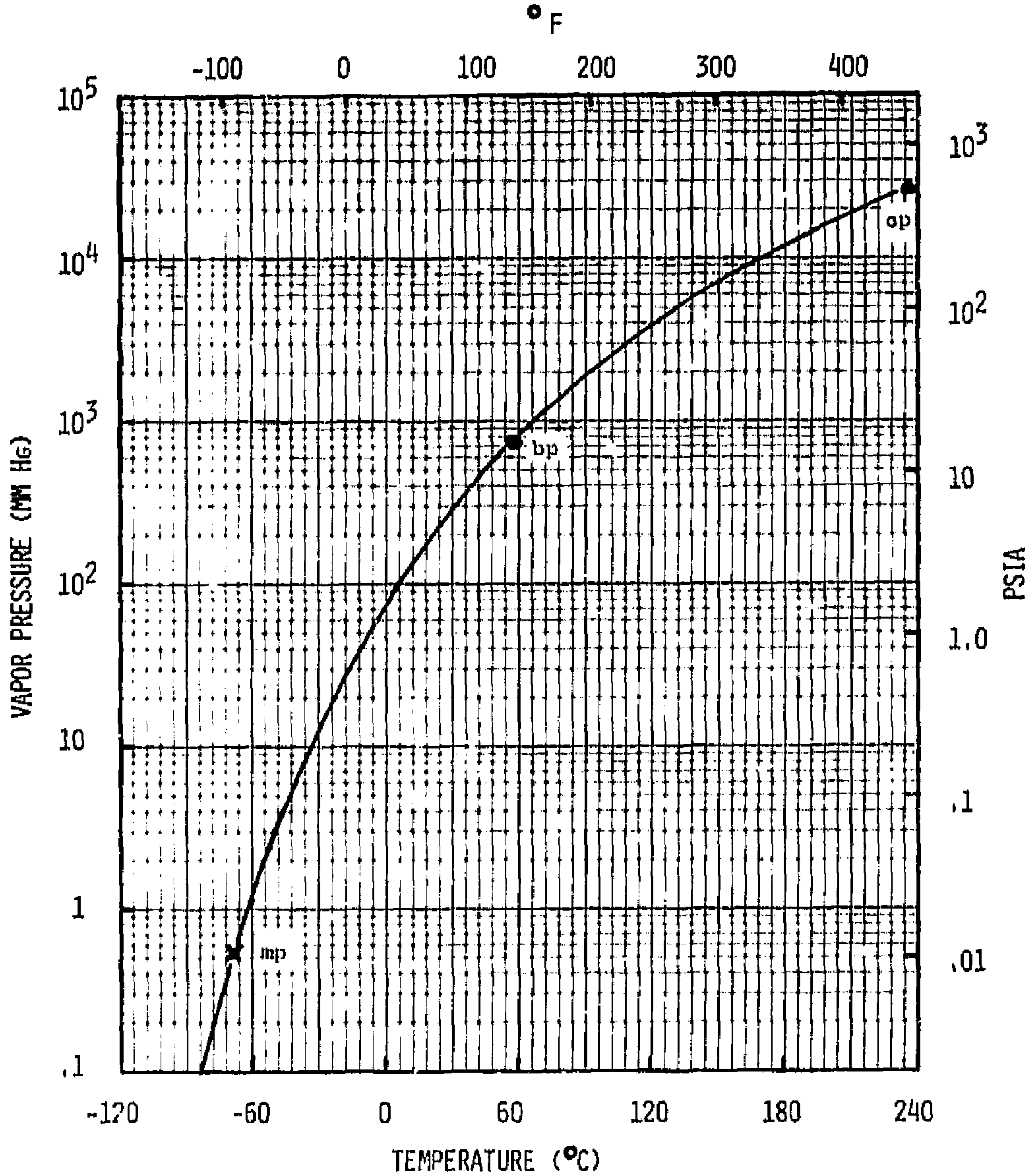

Figure 2.2-1 Vapor Pressure vs Temperature for Silicon Tetrachloride

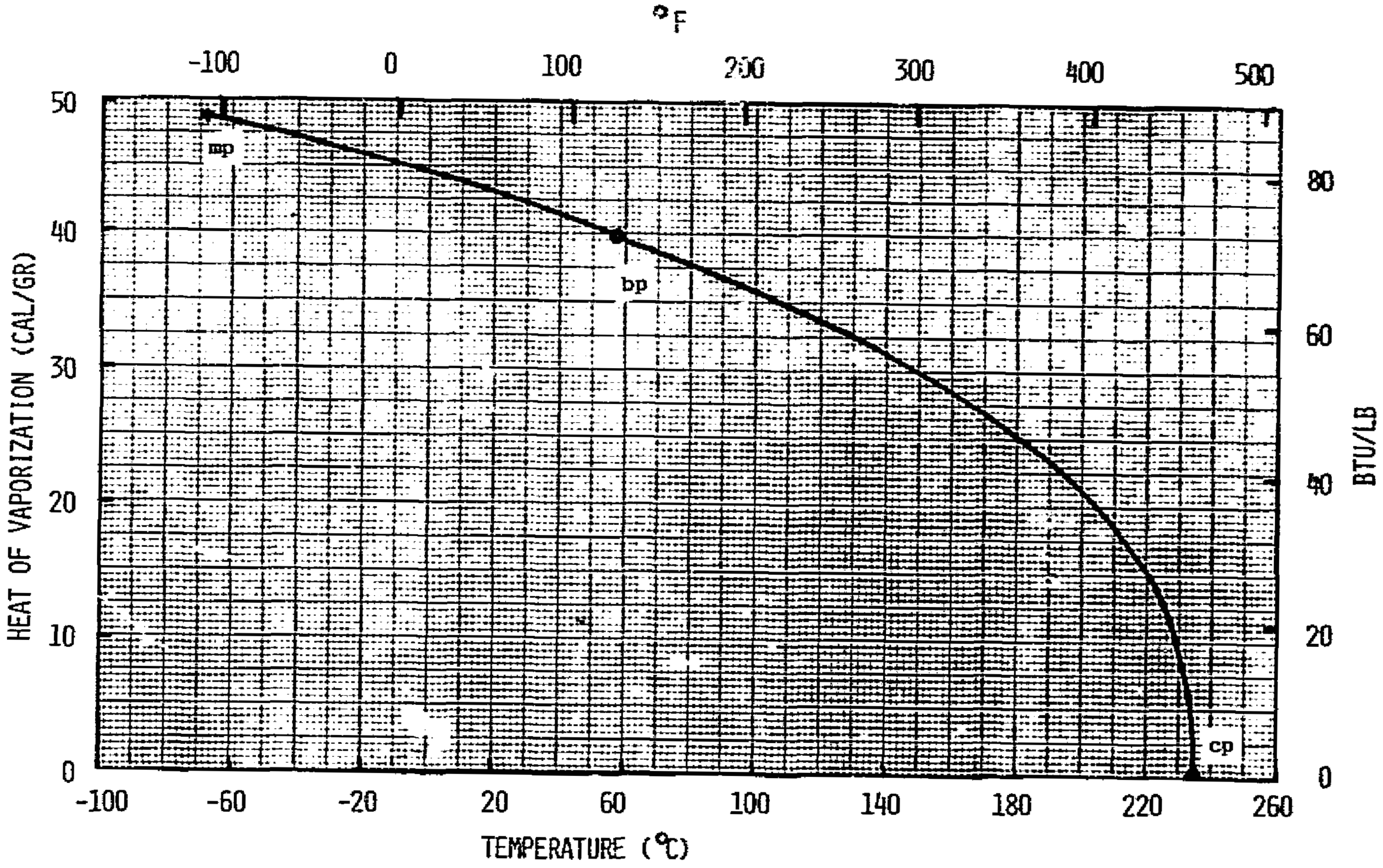

Figure 2.2-2 Heat of Vaporization vs Temperature for Silicon Tetrachloride

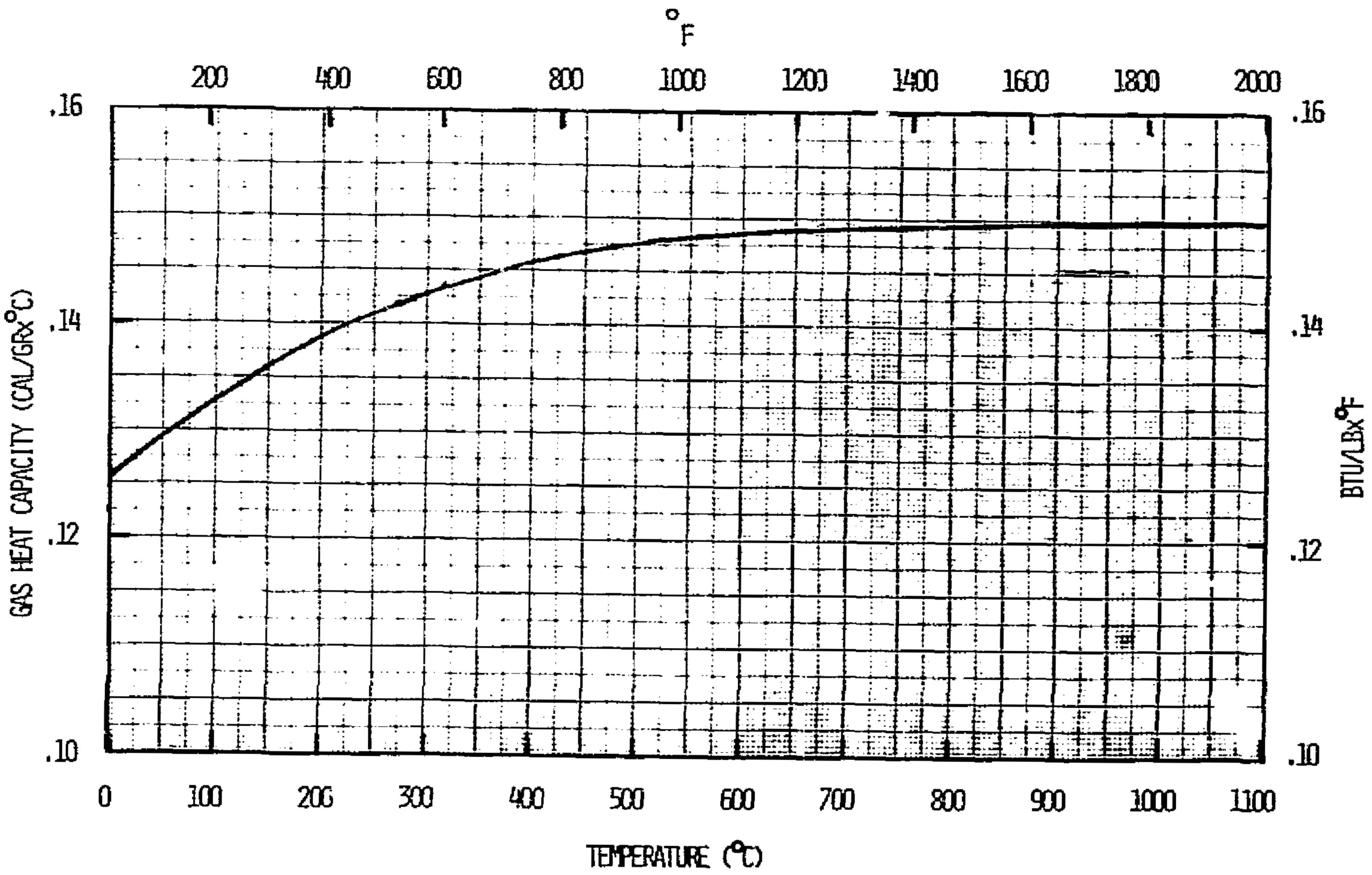

Figure 2.2-3 Gas Heat Capacity vs Temperature for Silicon Tetrachloride

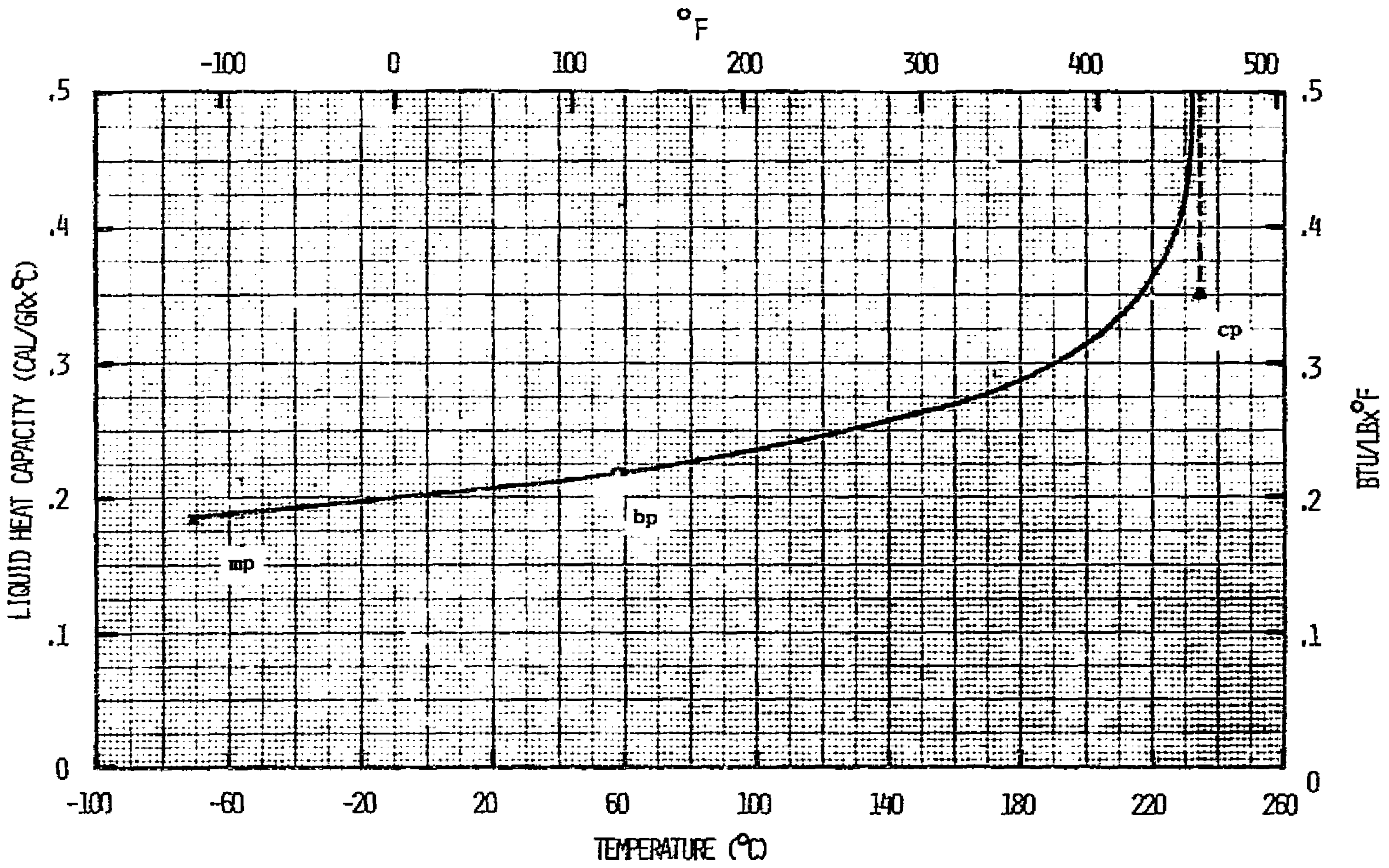

Figure 2.2-4 Liquid Heat Capacity vs Temperature for Silicon Tetrachloride

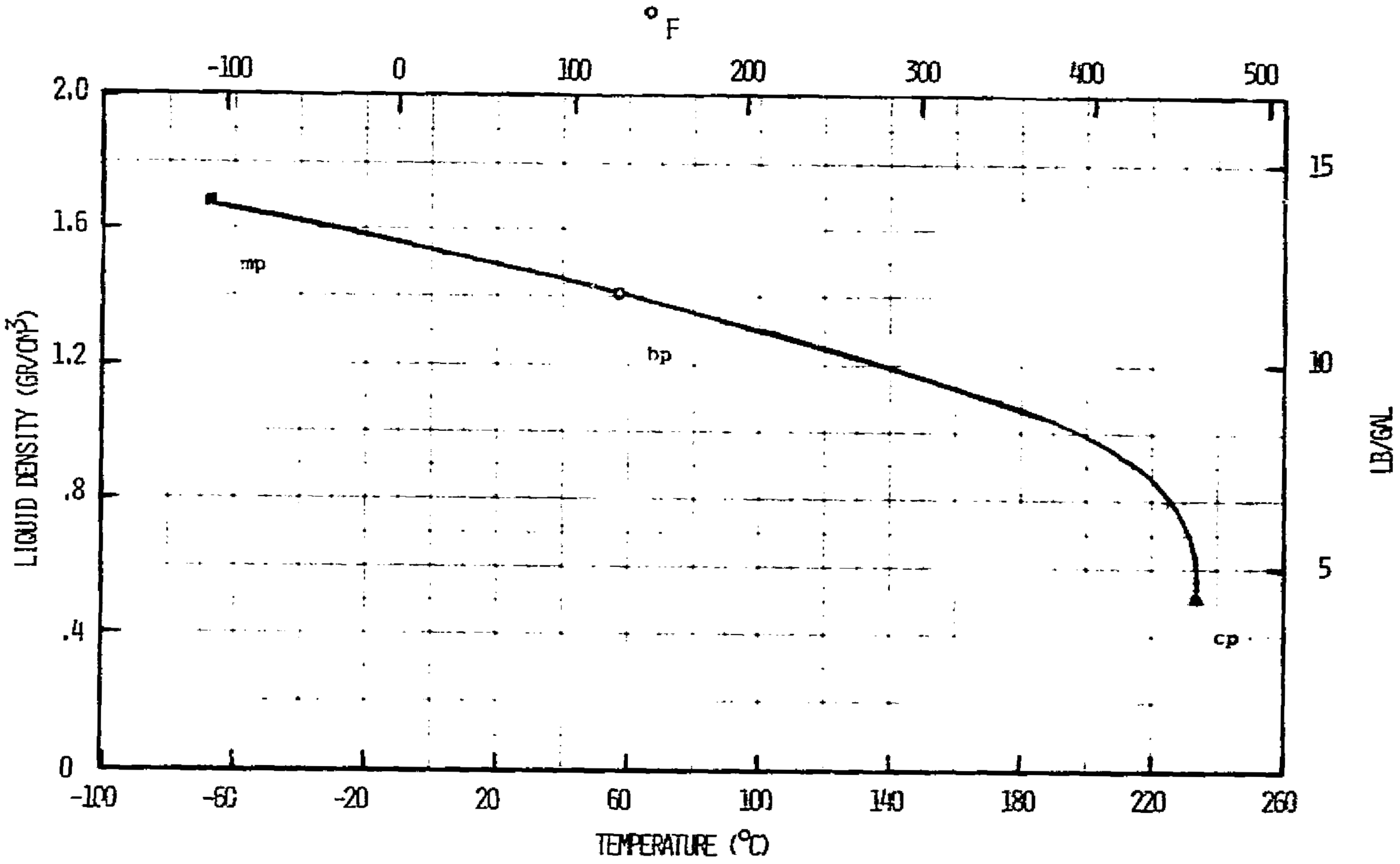

Figure 2.2-5 Liquid Density vs Temperature for Silicon Tetrachloride

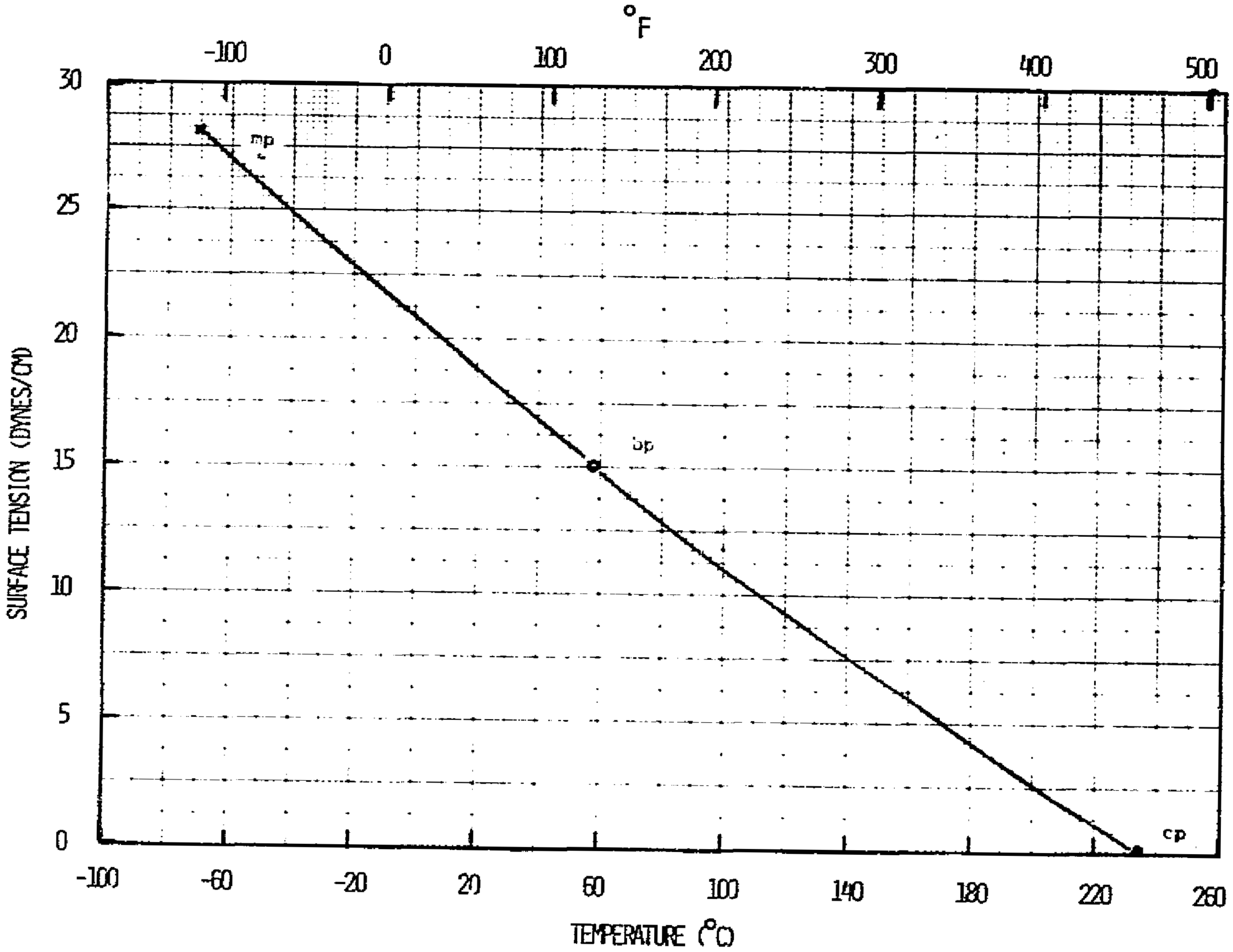

Figure 2.2-6 Surface Tension vs Temperature for Silicon Tetrachloride

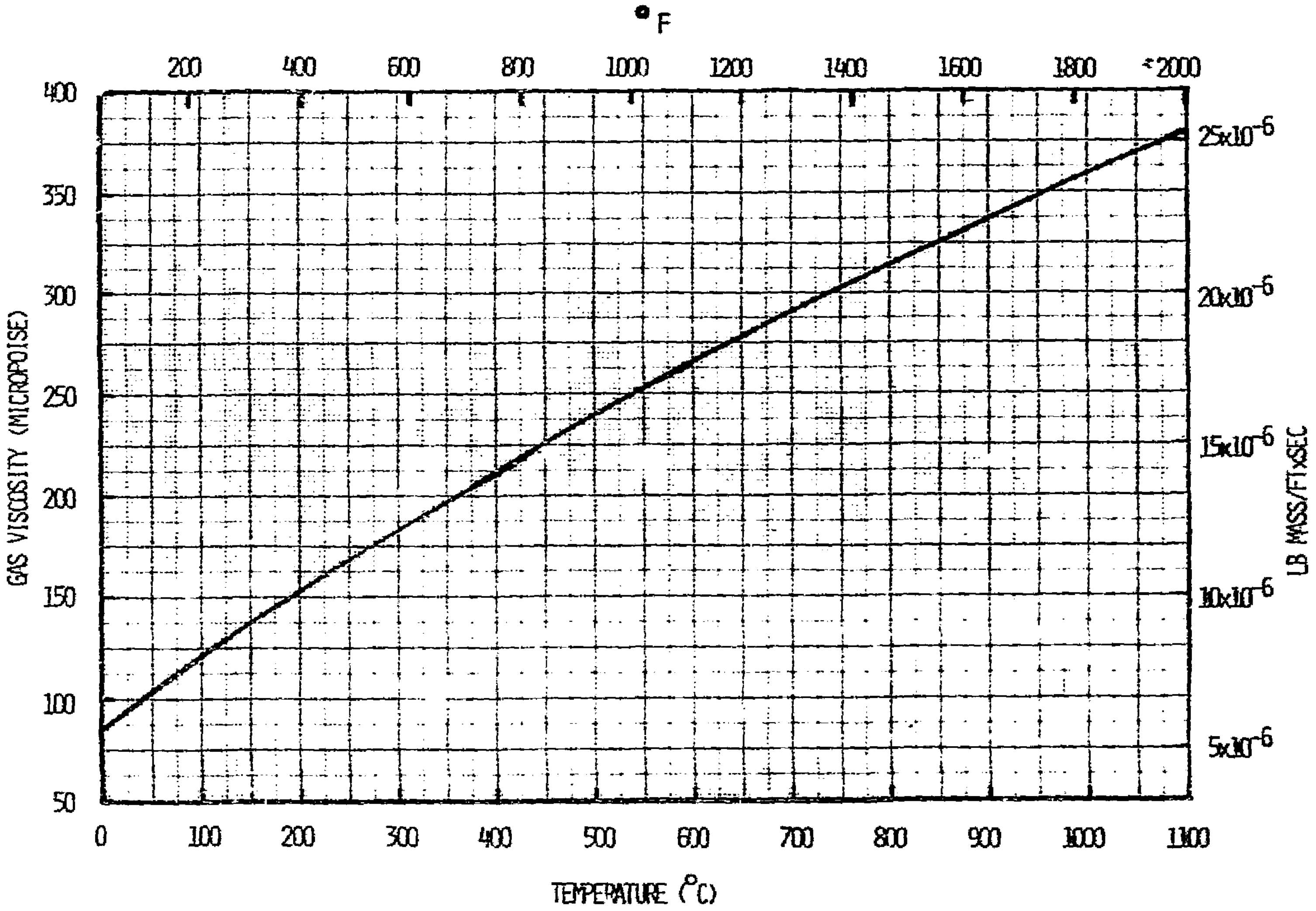

Figure 2.2-7 Gas Viscosity vs Temperature for Silicon Tetrachloride

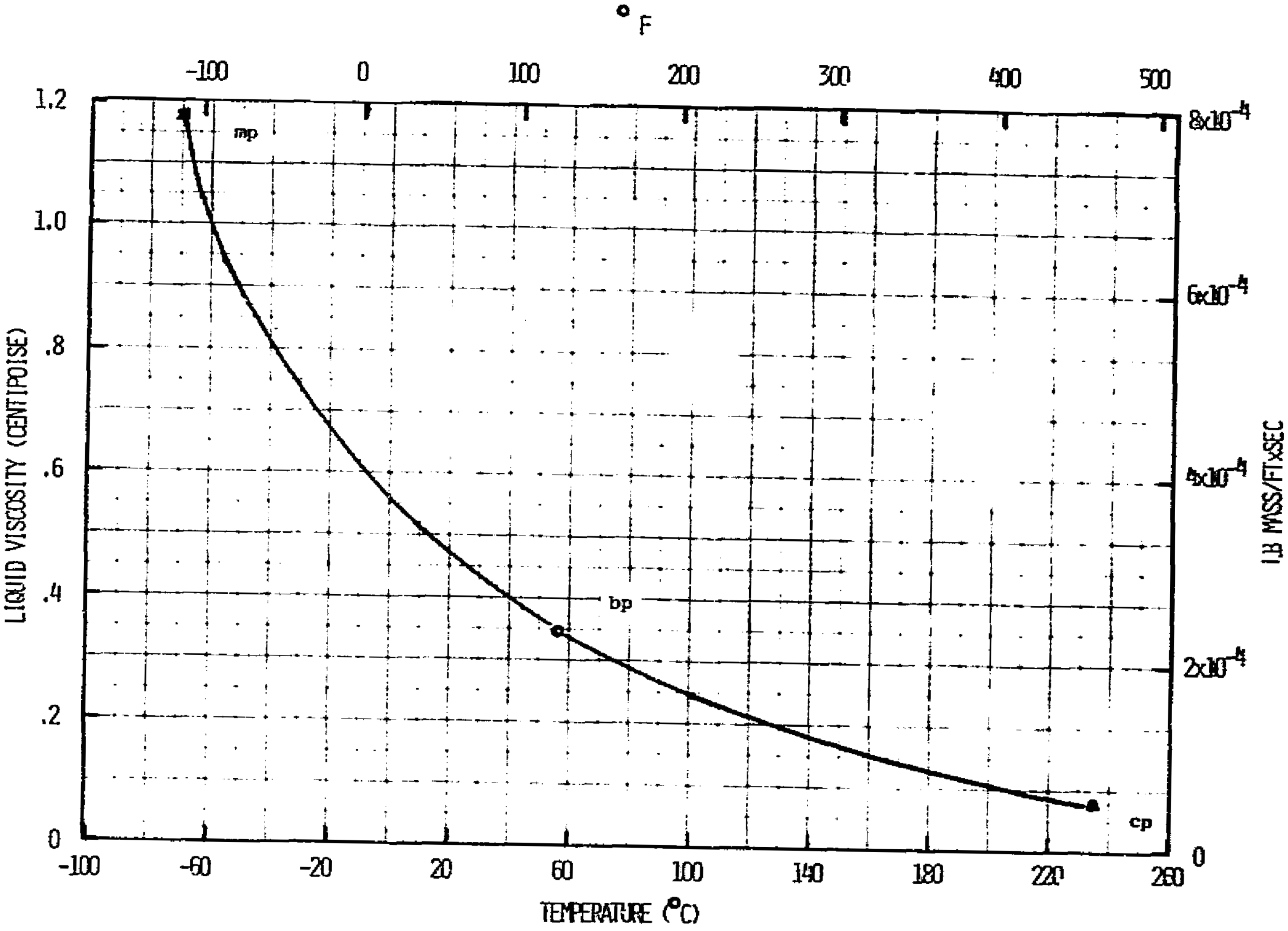

Figure 2.2-8 Liquid Viscosity vs Temperature for Silicon Tetrachloride

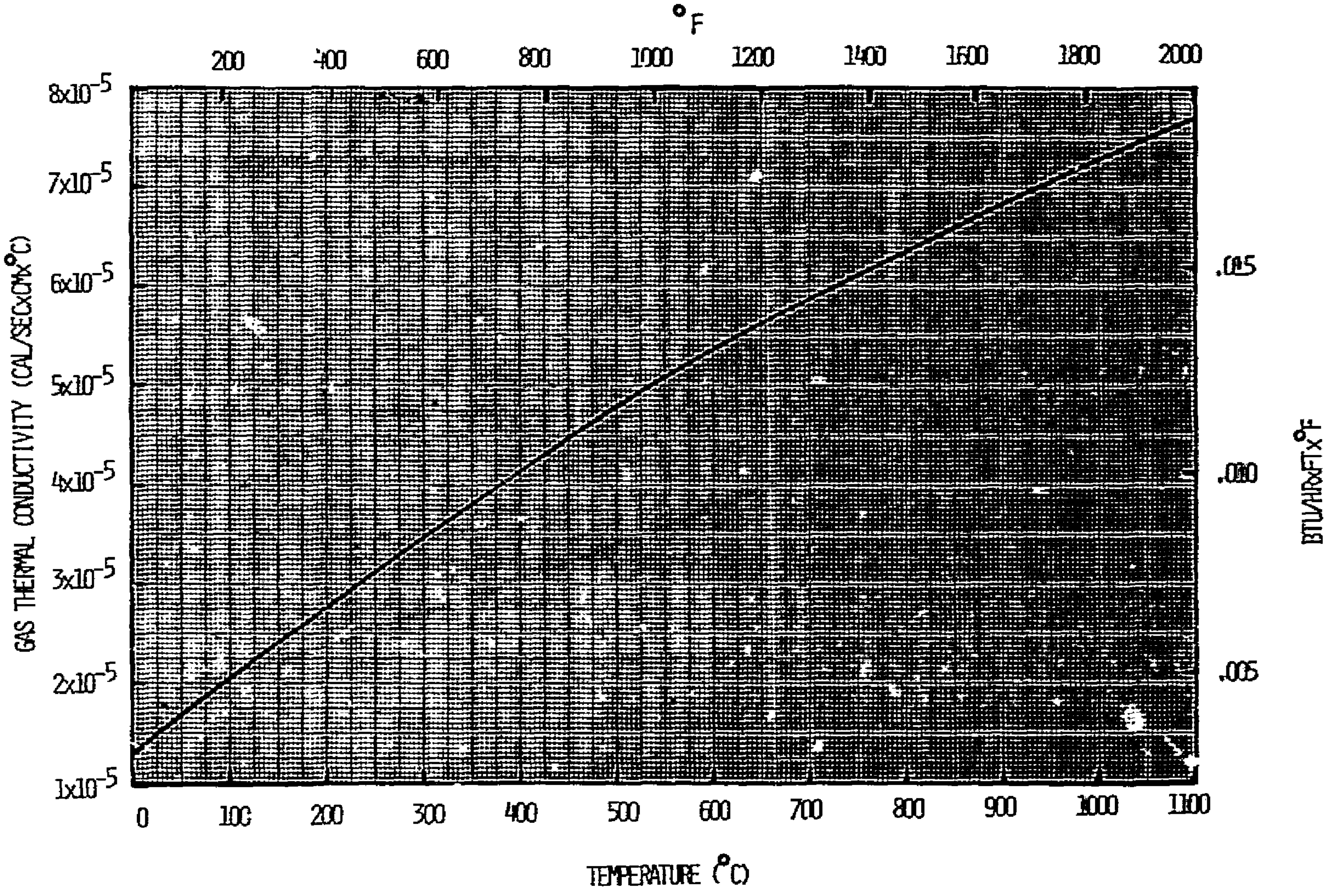

Figure 2.2-9 Gas Thermal Conductivity vs Temperature for Silicon Tetrachloride

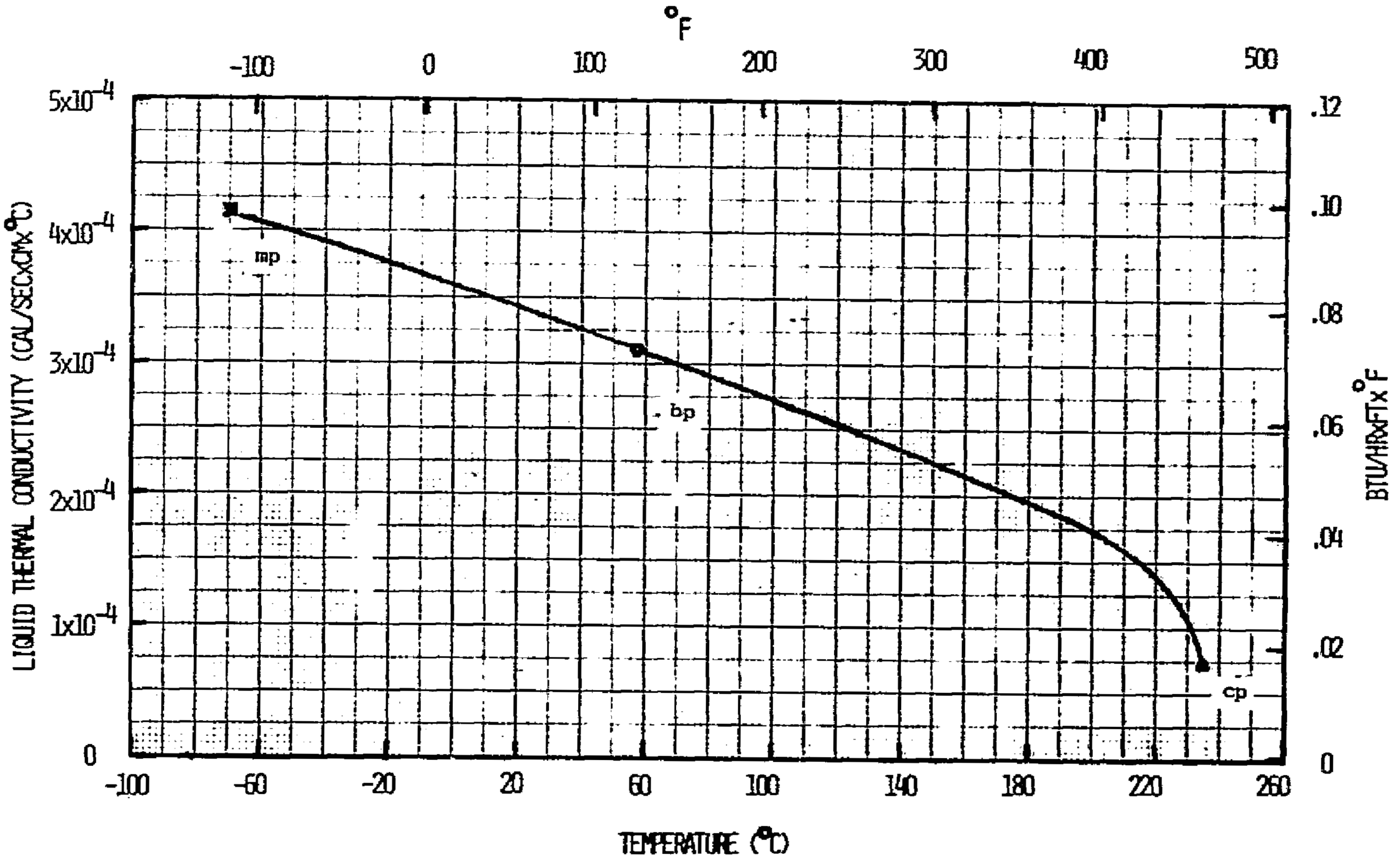

Figure 2.2-10 Liquid Thermal Conductivity vs Temperature for Silicon Tetrachloride

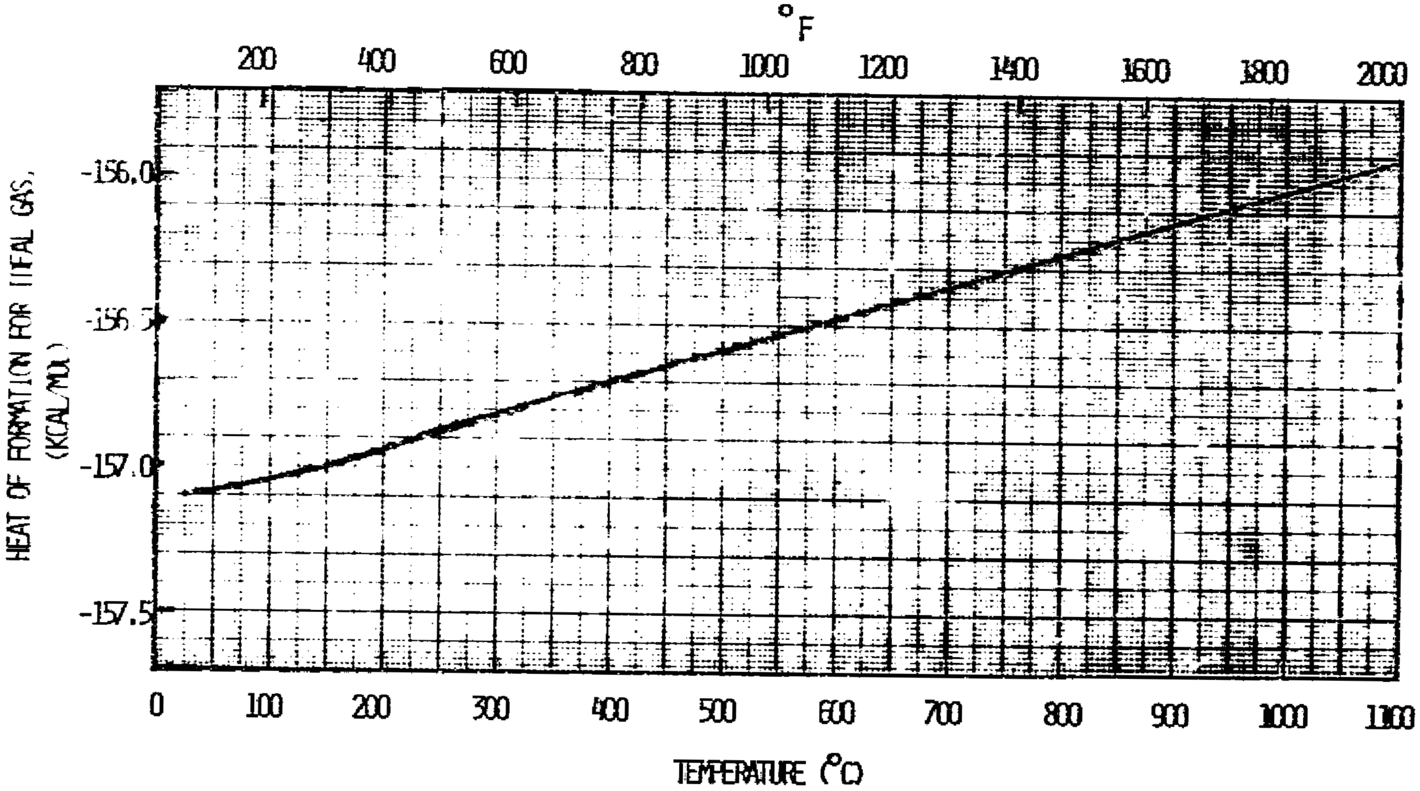

Figure 2.2-11 Heat of Formation vs Temperature for Silicon Tetrachloride

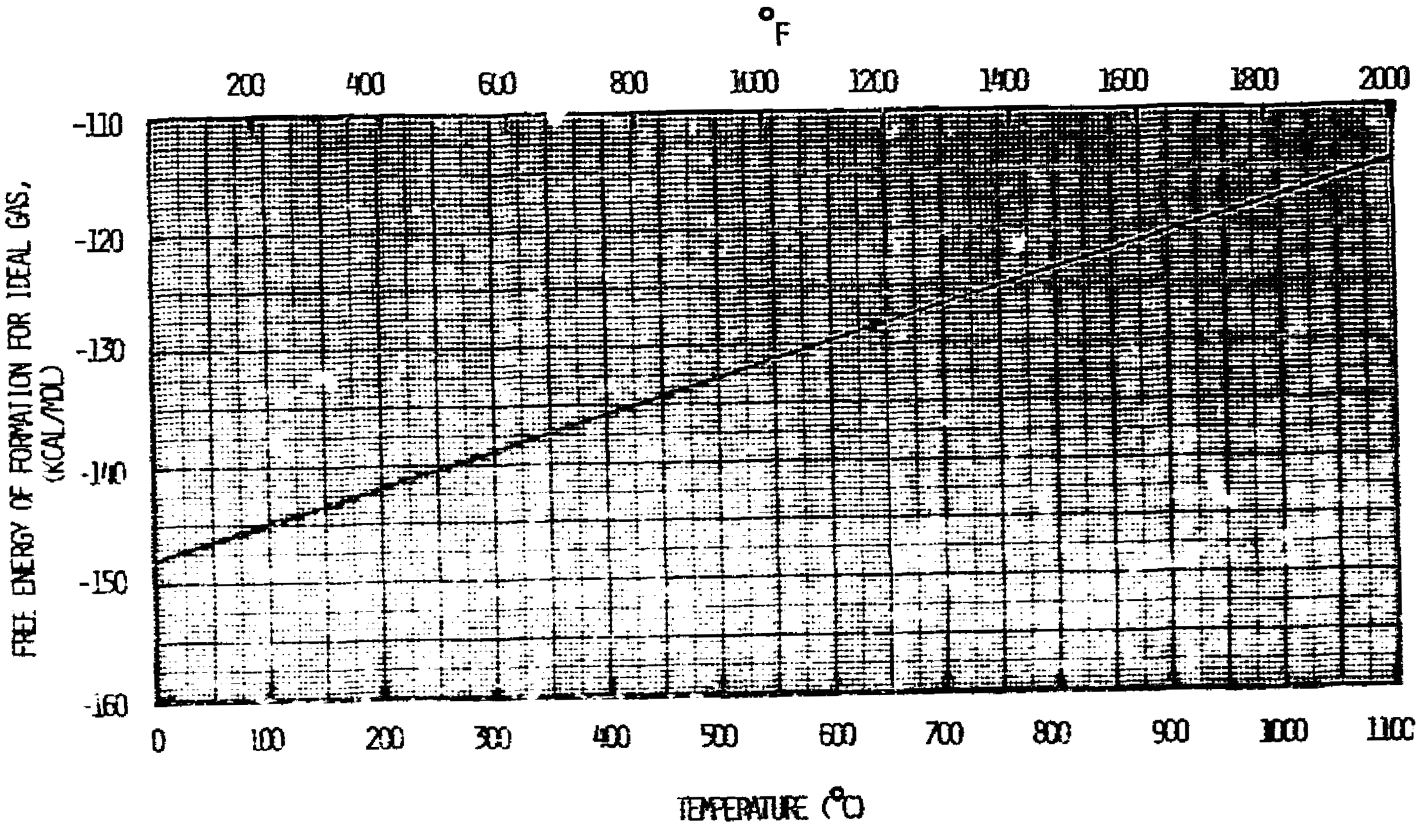

Figure 2.2-12 Free Energy of Formation vs Temperature for Silicon Tetrachloride

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2.3 Trichlorosilane Properties

Critical Properties (Table 2.3-1)

Experimental data for the critical temperature and critical volume are available (G33, G28) from a Russian investigation of orthobaric densities and critical paramaters. The critical pressure for trichlorosilane was estimated by Lydersen method (G62, G67):

$$P_c = \frac{M}{(\Sigma\Delta p + 0.34)^2} \qquad (2.3\text{-}1)$$

where P_c is critical pressure (atm), M is molecular weight (gr/gr-mol), and Δp is critical property increments for atoms making up the molecule. This method produced only 1.6% error when compared with the experimentally determined critical pressure of silicon tetrachloride.

The critical compressibility factor, Z_c, was calculated form its definition:

$$Z_c = \frac{P_c V_c}{R\ T_c} \qquad (2.3\text{-}2)$$

Vapor Pressure (Figure 2.3-1)

Observed vapor pressure data from several sources (G15, G29, G44, G61) for trichlorosilane are in general agreement from -85°C to just above the boiling point. The experimental data were extended to cover the entire liquid phase using the YSSP correlation relation (G63):

$$\log P_V = A + \frac{B}{T} + C \log T + DT \qquad (2.3\text{-}3)$$

where

P_V = vapor pressure of saturated liquid, mm of Hg

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

T = temperature, °K

The deviation of experimental and correlation results was small at 0.8% error for the 36 available data points.

Heat of Vaporization (Figure 2.3-2)

Heat of vaporization data for trichlorosilane are available only at the boiling point (G25, G18, G38, G46, G27). Using the known value at the boiling point, Watson's correlation (G62) was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_v = \Delta H_{v1} \left[\frac{T_c - T}{T_c - T_1} \right]^n \qquad (2.3\text{-}4)$$

where $n = .38$ and ΔH_{v1} applies at the boiling point (T_1).

Heat Capacity (Figures 2.3-3 and 2.3-4)

Heat capacity of the ideal gas at low pressure has been calculated by various Russian (G23, G25, G45, G11), American (G53, G56) and other (G6, G30) workers. The values, taken from various structural and spectral data, are in close agreement. The JANAF values (G53) were selected.

The liquid heat capacity of trichlorosilne is reported to be .23 between 25 and 60°C (G19, G46). The values are extended over all liquid temperatures by the relationship:

$$\text{Heat Capacity} \times \text{Density} = \text{Constant} \qquad (2.3\text{-}5)$$

The constant, C., was estimated to be 0.298.

Testing of this relaitonship with available data for silicon tetrachloride produced an average deviation of 4%.

Liquid Density (Figure 2.3-5)

Liquid density data for trichlorosilane are available from -10°C to the critical point(G33, G32, G61, G12, G26). The experimental data was extrapolated to the melting point by use of the Yaws-Shah relationship (G63) for saturated liquid:

$$\rho_L = AB^{-(1-T_r)^{2/7}} \qquad (2.3\text{-}6)$$

where $A = .4856$ and $B = .2618$. Correlation values and experimental results were in close agreement. The deviation was less than 1% for the [illegible] published data points from several independent sources.

Surface Tension (Figure 2.3-6)

Data for the surface tension of trichlorosilane are available from 0°C to 40°C (G32, G26). These data were extended using the Othmer relations (G62):

$$\sigma = \sigma_1 \left[\frac{T_c - T}{T_c - T_1} \right]^n \qquad (2.3\text{-}7)$$

where σ_1 = surface tension at T_1, dynes/cm, and n = the correlation parameter, 1.2. The other parameters have their usual meaning. Deviations between data and correlation values were 3% or less, largely due to the deviations between reported experimental values.

Viscosity (Figures 2.3-7 and 2.3-8)

Data for the gas viscosity of trichlorosilane were available only at 0°C and at boiling point (G25). The values at higher temperatures were estimated using the modified and revised corresponding-state method of Thodos and Yoon (G67, G68):

$$\eta_G \xi = 4.610\, T_r^{0.618} - 2.04\, e^{-0.-449 T_r} + 1.94\, e^{-4.058 T_r} + 0.1 \qquad (2.3\text{-}8)$$

where η_G = viscosity, $\xi = T_c^{1/6} M^{-1/2} P_c^{-2/3}$, and T_r is the reduced temperature. The percentage error was less than .4%. Testing with silicon tetrachloride gave good agreement of correlation and experimental results (16 data points produced a 2% deviation).

Liquid viscosity data for trichlorosilane are available from -7°C to 60°C (G32, G26, G19, G25, G46). At low temperatures (from the boiling to the melting point), values were estimated using the log η_L vs 1/T linear relationship. At high temperatures (up to the critical point), the Stiel and Thodos correlation was used with $\mu_L \xi = f(Z_c, T_r)$ where $f(Z_c, T_r)$ is given as a generalized liquid viscosity correlation (G62). The percentage error with the available experimental data was about 2%.

Thermal Conductivity (Figures 2.3-9 and 2.3-10)

The gaseous thermal conductivity of trichlorosilane has recently been reported from 46°C to 350°C (G66). The experimental values were extended using a modified form of the Misic and Thodos correlation (G63, G67):

$$\lambda_G = C_p/\gamma \ (10^{-6})(14.52 \ T_r - 5.14)^n \qquad (2.3\text{-}9)$$

where n = .71. The average absolute percentage error was 1.5%.

Liquid thermal conductivity data for trichlorosilane are not available. Using the estimation method of Sheffy and Johnson (G62):

$$\lambda_L = \{(4.66)(10^{-3})[1-.00126 \ (T - T_m)]/T_m^{.216} M^{.300}\} \qquad (2.3\text{-}10)$$

λ_L = 2.783 x 10^{-4} cal/cm x sec x °K was derived for the value at 60°C.

Using the Pachaiyappan-Vaidyanathan method of estimation (G64):

$$\lambda_L = 8.84 \times 10^{-4} \ C_p \ \rho_L \qquad (2.3\text{-}11)$$

the value of 2.64 x 10^{-4} cal/cm x sec x °K was derived for 60°C.

These estimation methods produced errors of 16% and 17.5%, respectively, on the one published value for $SiCl_4$; and hence, should be taken to represent only an order of magnitude estimate. The estimate was extended over the entire liquid range using a modification of the Stiel and Thodos method (G62, G63):

$$\lambda_L = \frac{f(\rho_r)}{\gamma Z_c^{5}} + \lambda_G \qquad (2.3\text{-}12)$$

Heat and Free Energy of Formation (Figures 2.3-11 and 2.3-12)

Values of the heat (ΔH_f) and Gibb's free energy of formation (ΔG_f) for the ideal gas are available from various Russian (G11, G45), American (G53) and other (G6, G30) sources and are in close agreement. The American values were selected.

TABLE 2.3-1

Critical Constants and Physical Properties of Trichlorosilane

Identification	Trichlorosilane
Formula	$SiHCl_3$
State (std. cond.)	liquid
Molecular Weight, M	135.453
Boiling Point, T_b, °C	31.8
Melting Point, T_m, °C	-126.6
Critical Temp., T_c, °C	206
Critical Pressure, P_c, atm	40.01*
Critical Volume, V_c, cm^3/gr mol	268
Critical Compressibility Factor, Z_c	.273*
Critical Density, ρ_c, gr/cm^3	.505
Acentric Factor (Ω)	.188*

*Estimated

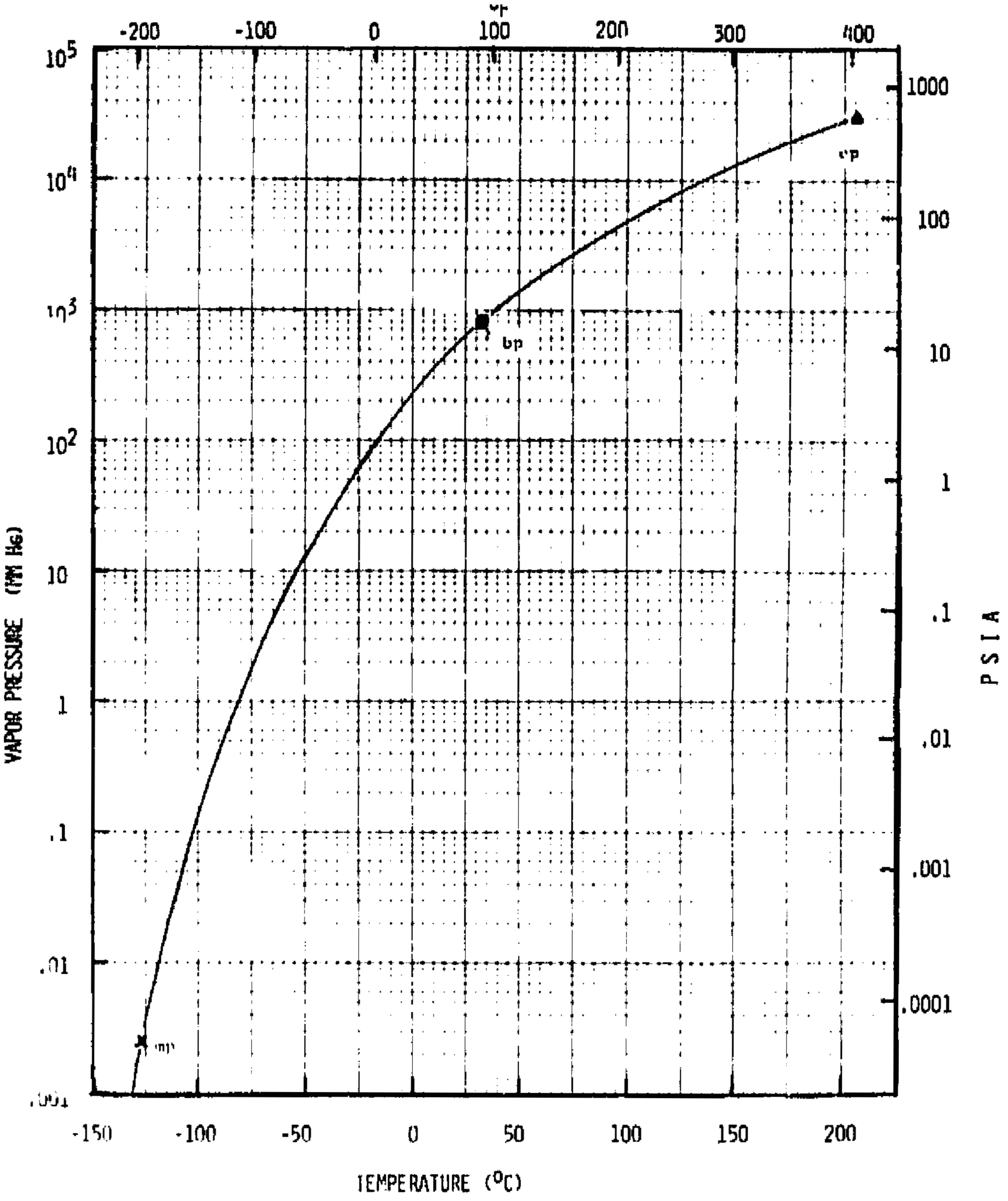

Figure 2.3-1 Vapor Pressure vs Temperature for Trichlorosilane

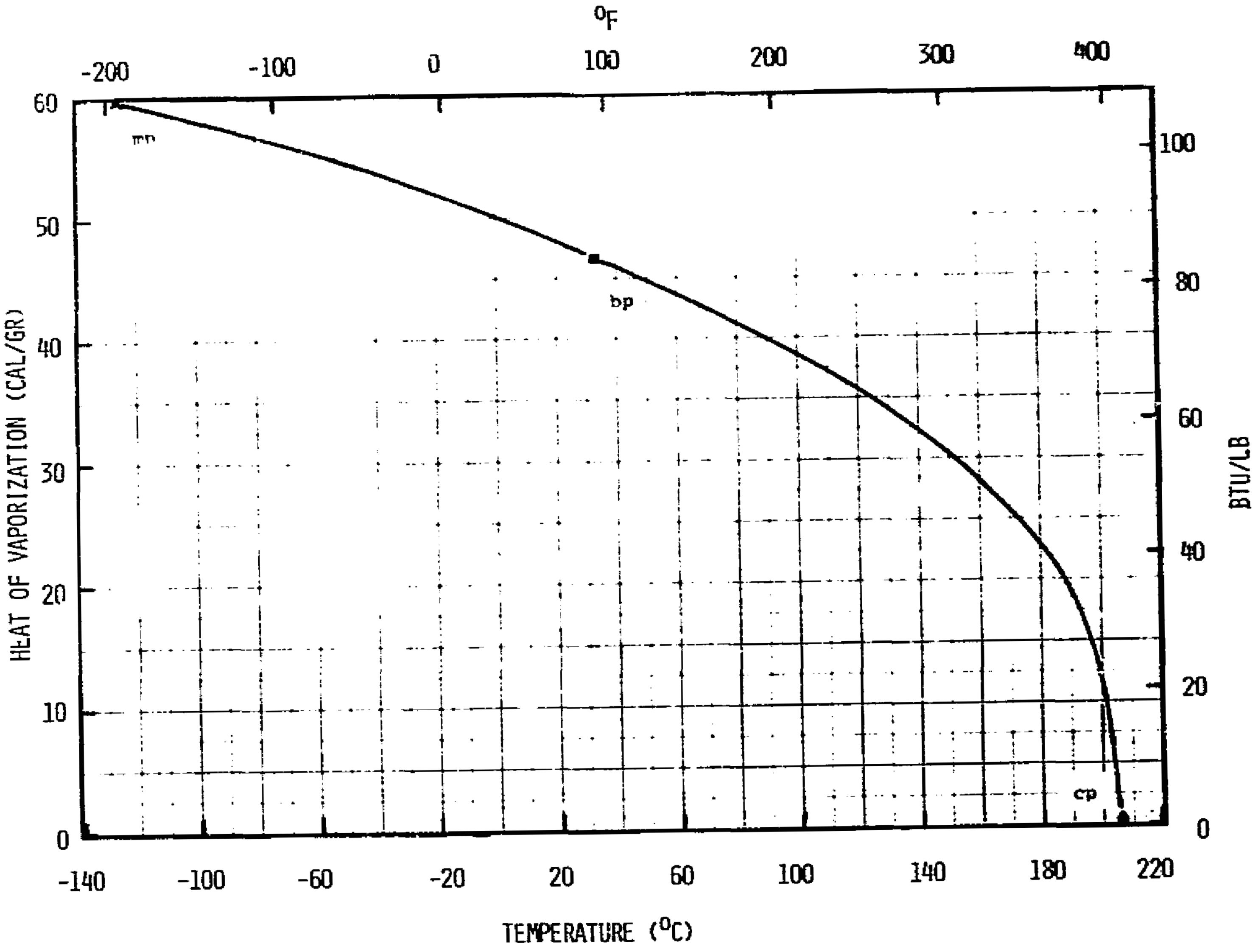

Figure 2.3-2 Heat of Vaporization vs Temperature for Trichlorosilane

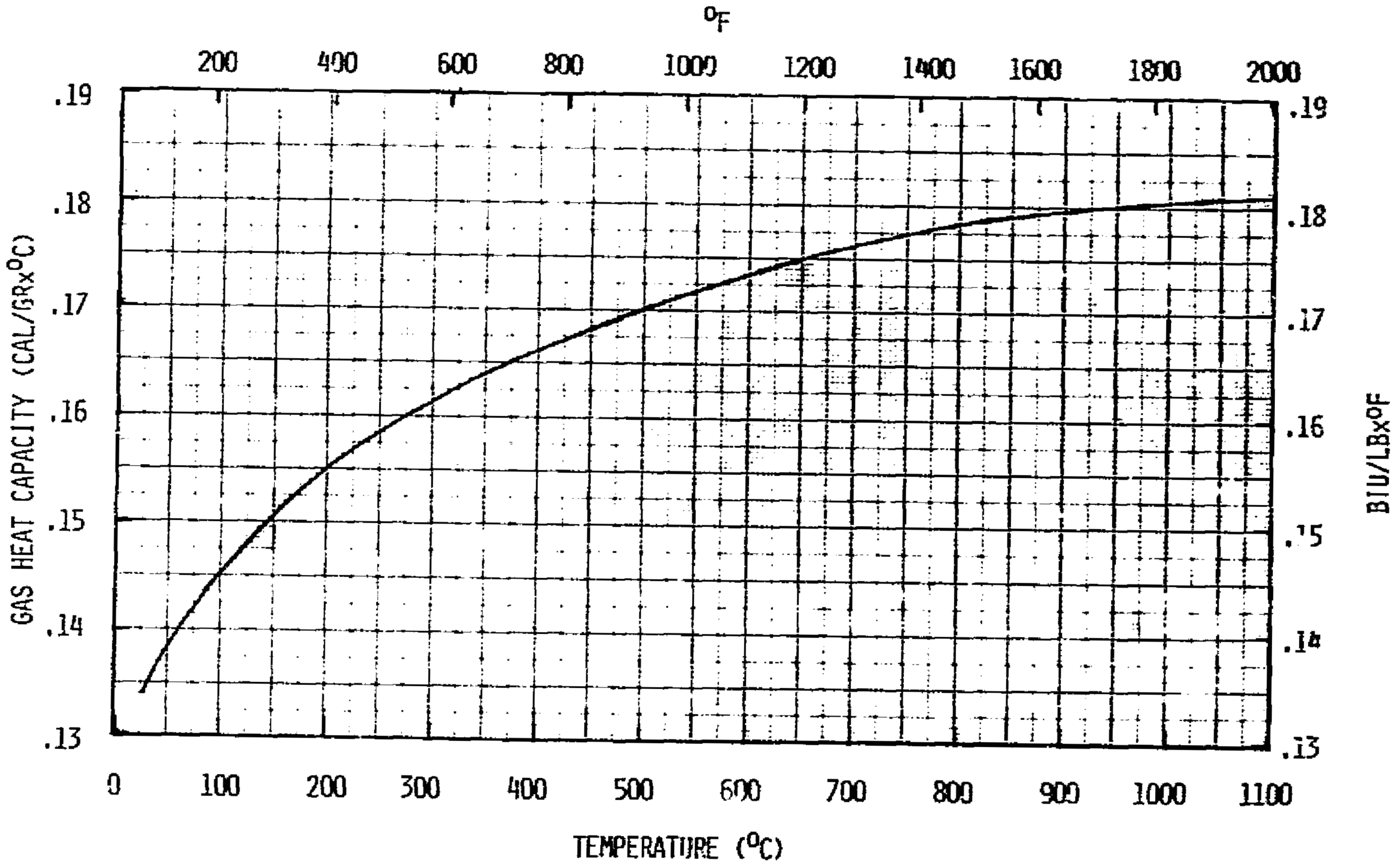

Figure 2.3-3 Gas Heat Capacity vs Temperature for Trichlorosilane

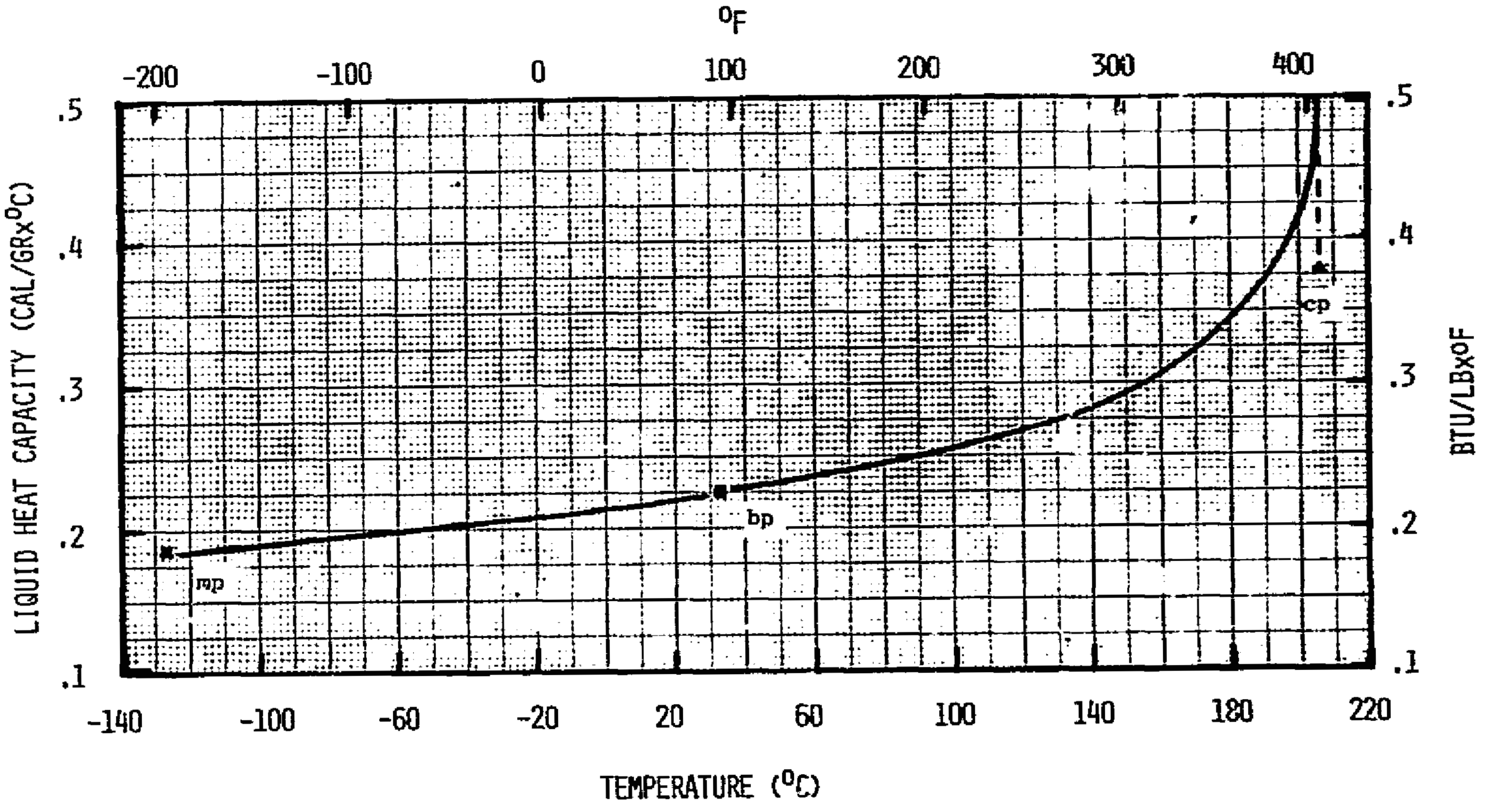

Figure 2.3-4 Liquid Heat Capacity vs Temperature for Trichlorosilane

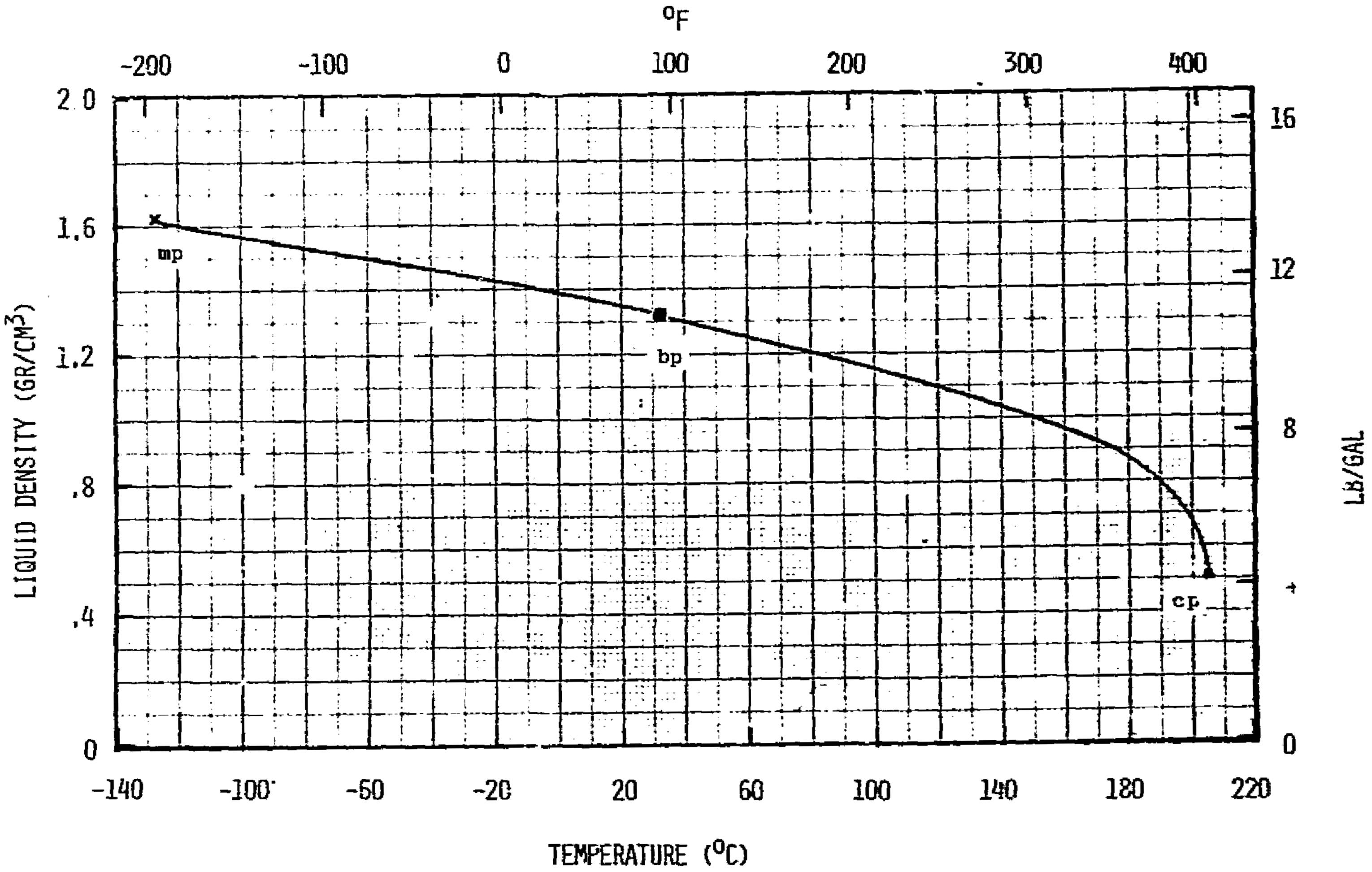

Figure 2.3-5 Liquid Density vs Temperature for Trichlorosilane

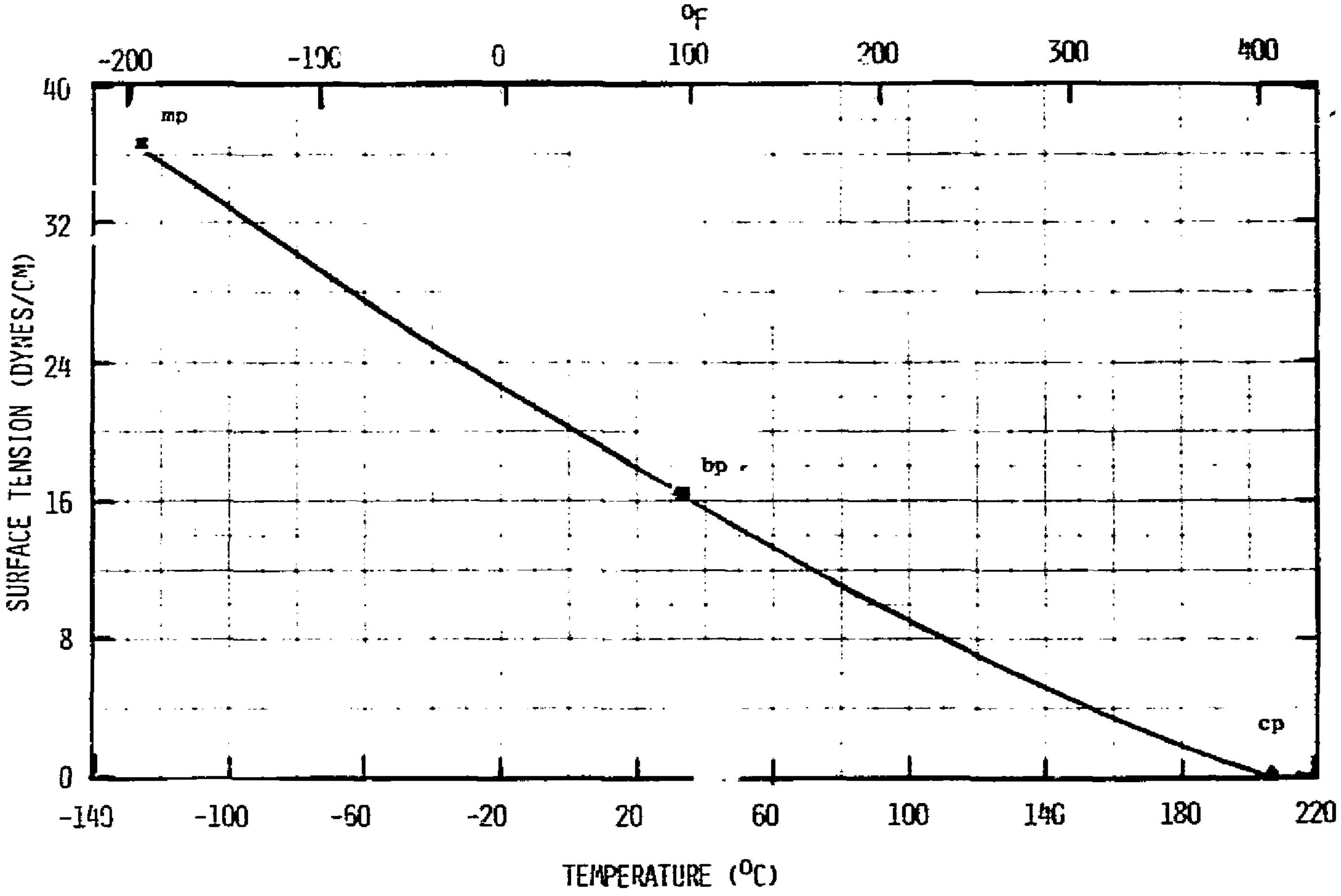

Figure 2.3-6 Surface Tension vs Temperature for Trichlorosilane

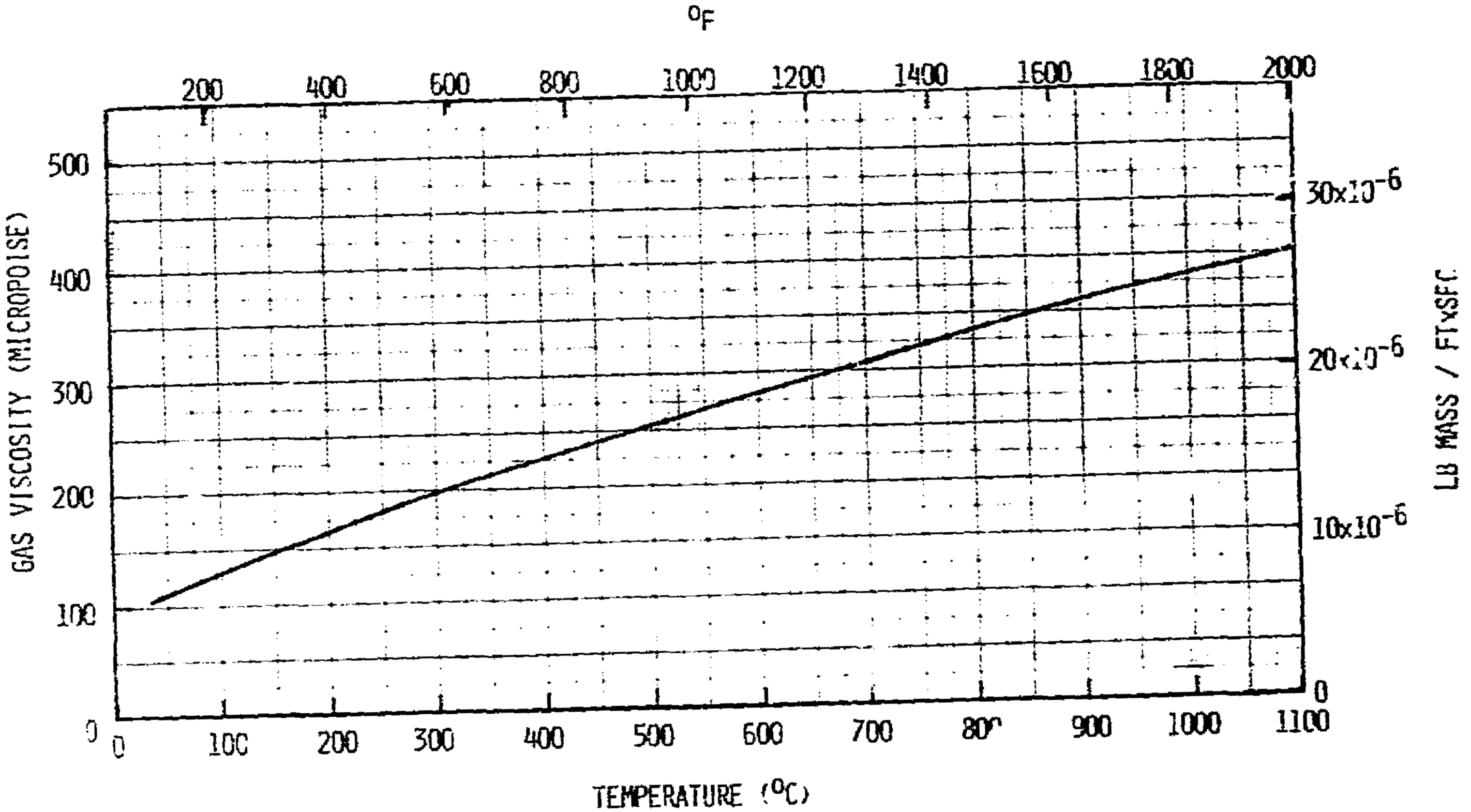

Figure 2.3-7 Gas Viscosity vs Temperature for Trichlorosilane

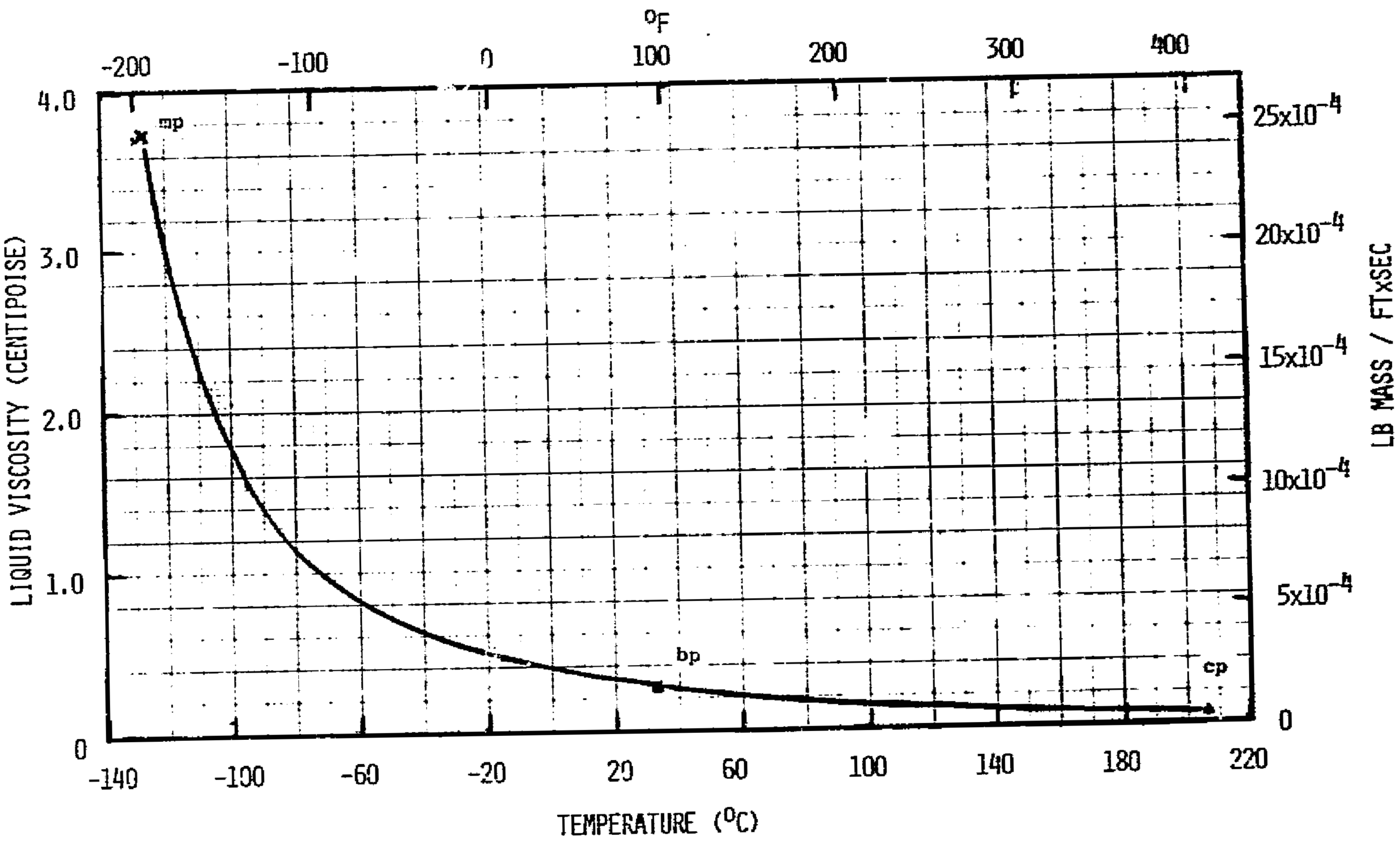

Figure 2.3-8 Liquid Viscosity vs Temperature for Trichlorosilane

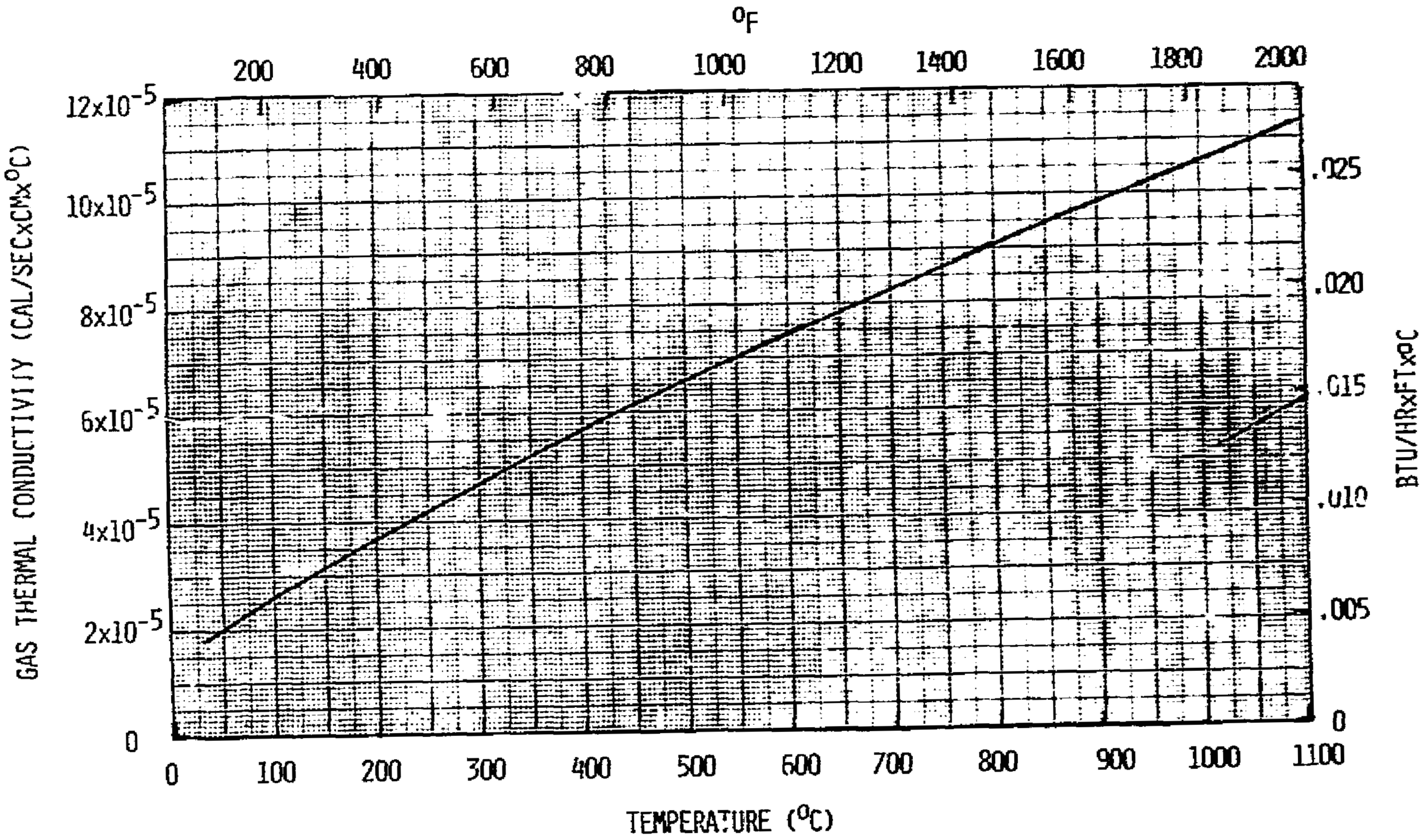

Figure 2.3-9 Gas Thermal Conductivity vs Temperature for Trichlorosilane

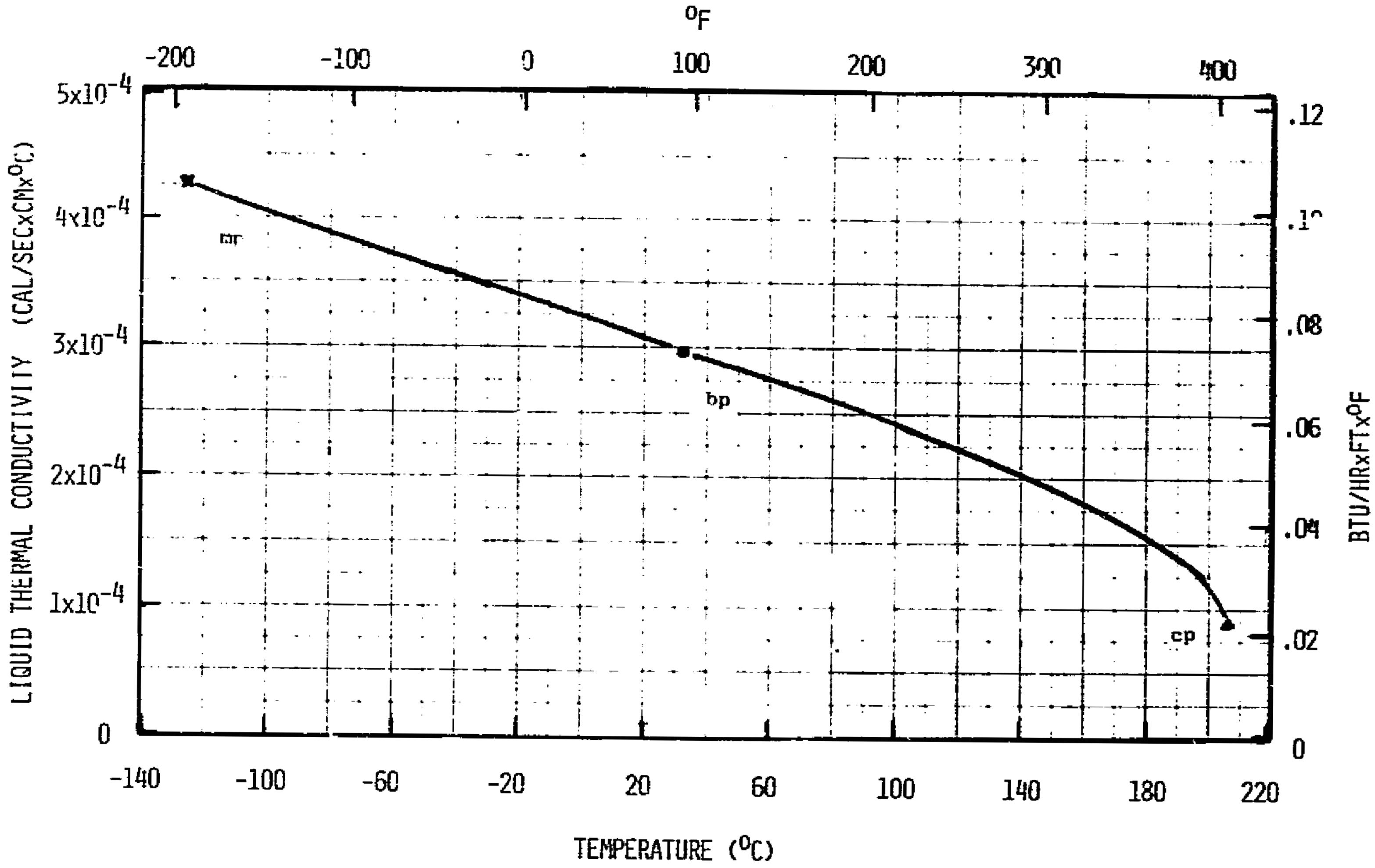

Figure 2.3-10 Liquid Thermal Conductivity vs Temperature for Trichlorosilane

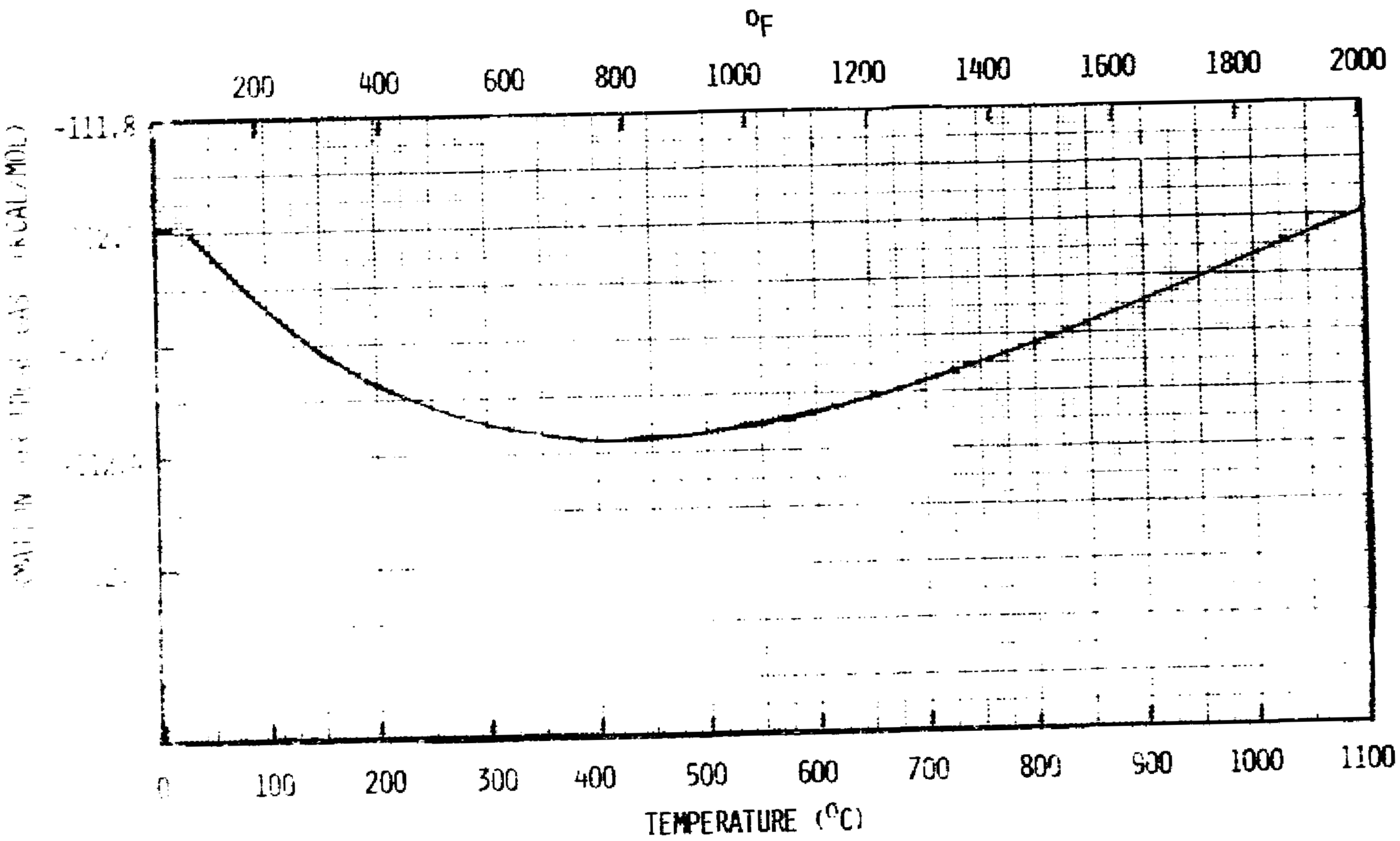

Figure 2.3-11 Heat of Formation vs Temperature for Trichlorosilane

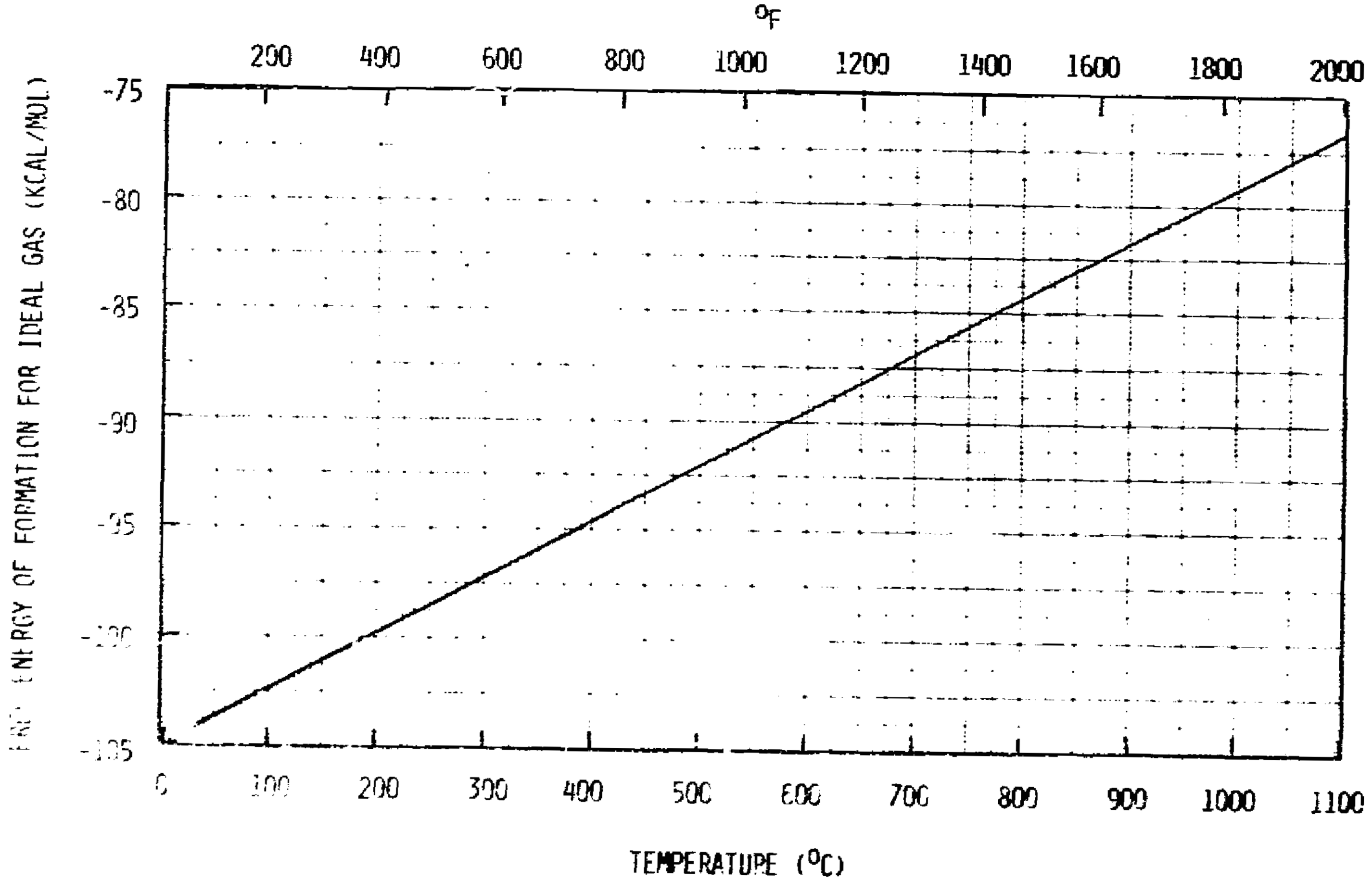

Figure 2.3-12 Free Energy of Formation vs Temperature for Trichlorosilane

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2.4 Dichlorosilane Properties

Physical Properties and Critical Constants (Table 2.4-1)

Physical properties and critical constants are listed in Table IA-1 for dichlorosilane. Values of critical temperature, T_c, critical pressure, P_c, and critical volume, V_c, for dichlorosilane were estimated by using Lydersen's structural contribution method with derived critical property increments for silicon (H16). This method produced only 2.3% error for T_c and 3.4% error for V_c when compared with the experimental values of trichlorosilane and it produced 0% error for T_c, V_c, and P_c when compared with the known values of silicon tetrachloride. The estimated values for the known values for the critical properties are also within reasonable agreement (4% for T_c, 0.2% for P_c, and 14% for V_c) of calculated Russian values (H10).

The critical compressibility factor, Z_c, was determined from its definition:

$$Z_c = \frac{V_c R T_c}{P_c} \tag{2.4-1}$$

The result from Eq. (IA-1) was the same as that derived by the Garcia-Barcena boiling point method (H16):

$$Z_c = f(T_b) - g(T_b/M) \tag{2.4-2}$$

Vapor Pressure (Figure 2.4-1)

The vapor pressure of dichlorosilane has been determined from -80°C to 30°C (H23, H35). The experimental data was extended over the entire liquid range using the YSSP vapor pressure correlation (H30):

$$\log P_V = A + \frac{B}{T} + C \log T + DT + ET^2 \tag{2.4-3}$$

where P_V is the vapor pressure of saturated liquid, mm Hg; T is temperature, °K; and A, B, C, D, E are correlation constants derived using a generalized least squares computer program. Average absolute deviation was about 1% for the 13 experimental data points.

Heat of Vaporization (Figure 2.4-2)

Heat of vaporization data for dichlorosilane are available only at the boiling point (H1, H0, H10, H19, H31). Using the known value at the boiling point, Watson's correlation was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_V = \Delta H_{V_1} \left[\frac{T_c - T}{T_c - T_1}\right]^n \qquad (2.4\text{-}4)$$

where n = .38 and ΔH_{V_1} applies at the boiling point (T_1).

Heat Capacity (Figures 2.4-3 and 2.4-4)

Ideal gas heat capacity data for dichlorosilane are available from various American (H5, H13, H25, H26), Russian (H6, H7, H10, H12, H32) and other (H9, H33) workers. The vlaues, which are in close agreement, are based on bond additivities and spectral measurement. The JANAF values were selected.

Measured saturated-liquid heat capacity data for dichlorosilane are unavailable in the literature. Values were estimated from -60°C to 60°C using the Yuan and Stiel corresponding state method (H16). For polar liquids, the correlation takes the form:

$$C_{\sigma_1} - C_p^o = \Delta C^{(0p)} + \omega(\Delta C_\sigma)^{(1p)} + X(\Delta C_\sigma)^{(2p)} + X^2(\Delta C_\sigma)^{(3p)} + \omega^2(\Delta C_\sigma)^{(4p)} + X\omega\,(\Delta C_\sigma)^{(5p)} \qquad (2.4\text{-}5)$$

where C_p^o is the ideal gas heat capacity, ω is the acentric factor, X is the Stiel polar factor and the funcions: $(\Delta C_\sigma)^{(0p)}$, etc. are tabulated as functions of the reduced temperature. The relationship that heat capacity times density is constant was used to extend the values over the entire liquid range. Application of the Yuan and Stiel correlations to silicon tetrachloride, trichlorosilane, and silicon tetrafluoride gave average absolute percentage errors of 3.1, 6.7, and 4.3 respectively. Due to the limited experimental data points, the calculated liquid heat capacities should be considered as order-of-magnitude estimates.

Density (Figure 2.4-5)

Liquid density data are available at the melting point (H8, H9, H10, H18, H27) and at 7°C (H35). The limited data were extended over the entire liquid range using a modification of the Rackett equation:

$$\rho = \rho_c\, Z^{-(1-T_r)^{2/7}} \qquad (2.4\text{-}6)$$

where ρ_c is critical density, T_r is reduced temperature and Z is a parameter defined by the experimental data.

Surface Tension (Figure 2.4-6)

The Brock and Bird corresponding states method (H16) was used to estimate the surface tension of dichlorosilane since no experimental data is available. The equation is:

$$\sigma = P_c^{2/3} T_c^{1/3} (0.133\ \alpha_c - 0.281)(1 - T_r)^{11/9} \qquad (2.4\text{-}7)$$

where σ is surface tension, dynes/cm, α_c is the Riedel parameter, P_c is critical pressure, atm.; T_c is critical temperature, °K; and T_r is the reduced temperature. Application of this method to silicon tetrachloride and trichlorosilane gave results within 4% and 0.8% absolute deviation with experimental data, respectively.

Viscosity (Figures 2.4-7 and 2.4-8)

Gas viscosity calculations at low pressure were made using the methods of (1) Yoon and Thodos for non-hydrogen-bonding polar gases, (2) Golubev, and (3) Reichenberg (H16). Since the calculated values were in close agreement, they were fitted to the series expansion:

$$\eta_G = A + BT + CT^2 \qquad (2.4\text{-}8)$$

where η_G is in micropoise; T is temperature, °K; and A, B and C are computer derived parameters using a generalized least squares program. The average absolute percentage deviation was less than 1.8%.

Liquid viscosities at temperatures below the boiling point were calculated using the methods of Thomas, and of Morris (up to 60°C) (H16). Values from the boiling point to the critical point were calculated using the correlation methods of Letson and Stiel, and Stiel and Thodos (H16). Calculated values were extended over entire liquid range and fitted to the equation:

$$\log \eta_L = A + \frac{B}{T} + CT + DT^2 \qquad (2.4\text{-}9)$$

where η_L is in centipoise; T is temperature, °K; and A, B, D and D are derived parameters using a generalized least squares computer program. This was done in order to fit together the calculated values which apply in the different temperature ranges. The average percentage deviation was 3.3% with the greater deviation being near the melting point; therefore, this should be considered to be an order-of-magnitude correlation.

Thermal Conductivity (Figures 2.4-9 and 2.4-10)

Gas-phase thermal conductivity data are available from 28°C to 350°C (H28). The data were correlated and extended to higher temperatures by a series expansion in temperature:

$$\lambda_G = A + BT + CT^2 + DT^3 \qquad (2.4\text{-}10)$$

where λ_G is gas thermal conductivity, cal/cm x sec x °C; T is temperature, °K; and A, B, C and D are computer derived constants characteristic of the chemical compound. The absolute deviation between data and correlation values was less than 0.5%.

Thermal conductivity data of the liquid phase is unavailable. Modifications of the estimation methods of Sato and Reidel (H16):

$$\lambda_L = \frac{2.64 \times 10^{-3}}{M^{1/2}} \; \frac{3 + 20\,(1 - T_r)^{2/3}}{3 + 20\,(1 - T_{r_b})^{2/3}} \qquad (2.4\text{-}11)$$

and of Robbins and Kingrea (H15):

$$\lambda_L = \frac{(88 - 4.94\,H) \times 10^{-3}}{\Delta S^*} \; \frac{.55}{T_r} \; C_{p_L} \rho^{4/3} \qquad (2.4\text{-}12)$$

where used to derive values at 32°C. These modified estimation methods produced error of less than 1% absolute deviation on the one published value of $SiCl_4$. The average of the estimate at 32°C was extended over the entire liquid range using a modification of the Stiel and Thodos method (H16):

$$\lambda_L = \frac{f(\rho_r)}{\Gamma Z_c^{\,5}} + \lambda_G \qquad (2.4\text{-}13)$$

The modified Sato-Reidel equation produced a similar range of values. Since assumptions in these calculations include the accuracy of the one data point for silicon tetrachloride and the chemical similarities in a homologous series, these values should be considered only order-of-magnitude estimates.

Heat and Free Energy of Formation (Figures 2.4-11 and 2.4-12)

Heat of formation and Gibb's free energy of formation for the ideal gas have been estimated by Russian (H32, H36) and American (H25) workers up to at least 1500°K. Some estimated values differ significantly having about 35% deviation for ΔH_f and about 45% deviation for ΔG_f (H32, H36). The JANAF values (H25) were selected.

TABLE 2.4-1

CRITICAL CONSTANTS AND PHYSICAL PROPERTIES OF DICHLOROSILANE

Identification	Dichlorosilane
Formula	SiH_2Cl_2
State (std. cond.)	gas
Molecular weight, M	101.008
Boiling Point, T_b, °C	8.3
Melting Point, T_m, °C	-122.0
Critical Temperature, T_c, °C	178.9*
Critical Pressure, P_c, atm	44.0*
Critical Volume, V_c, cm^3/gr mol	228.3*
Critical Compressibility Factor, Z_c	.276*
Critical Density, ρ_c, gr/cm^3	.4424*
Acentric Factor (ω)	.1107

*Estimated

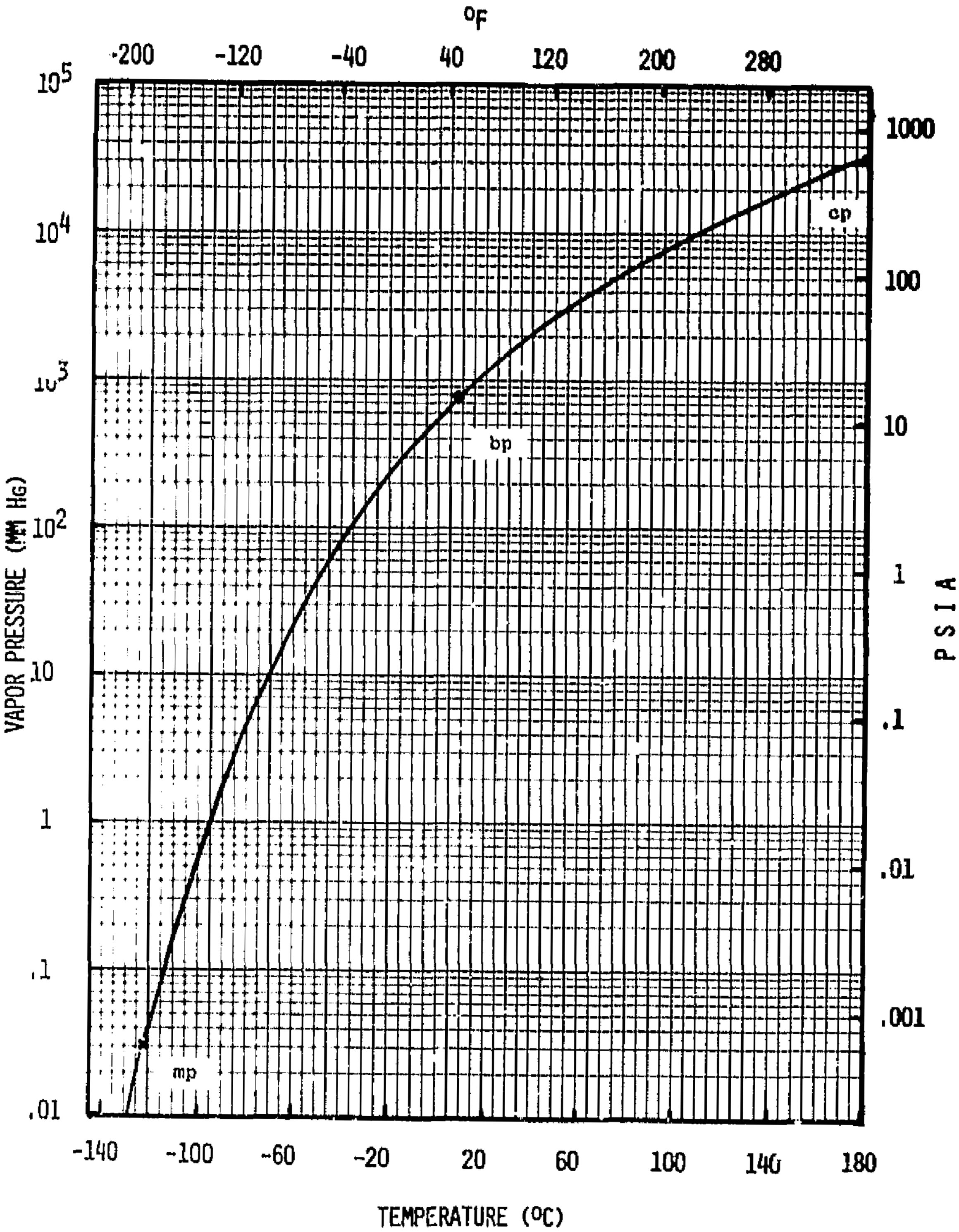

Figure 2.4-1 Vapor Pressure vs Temperature for Dichlorosilane

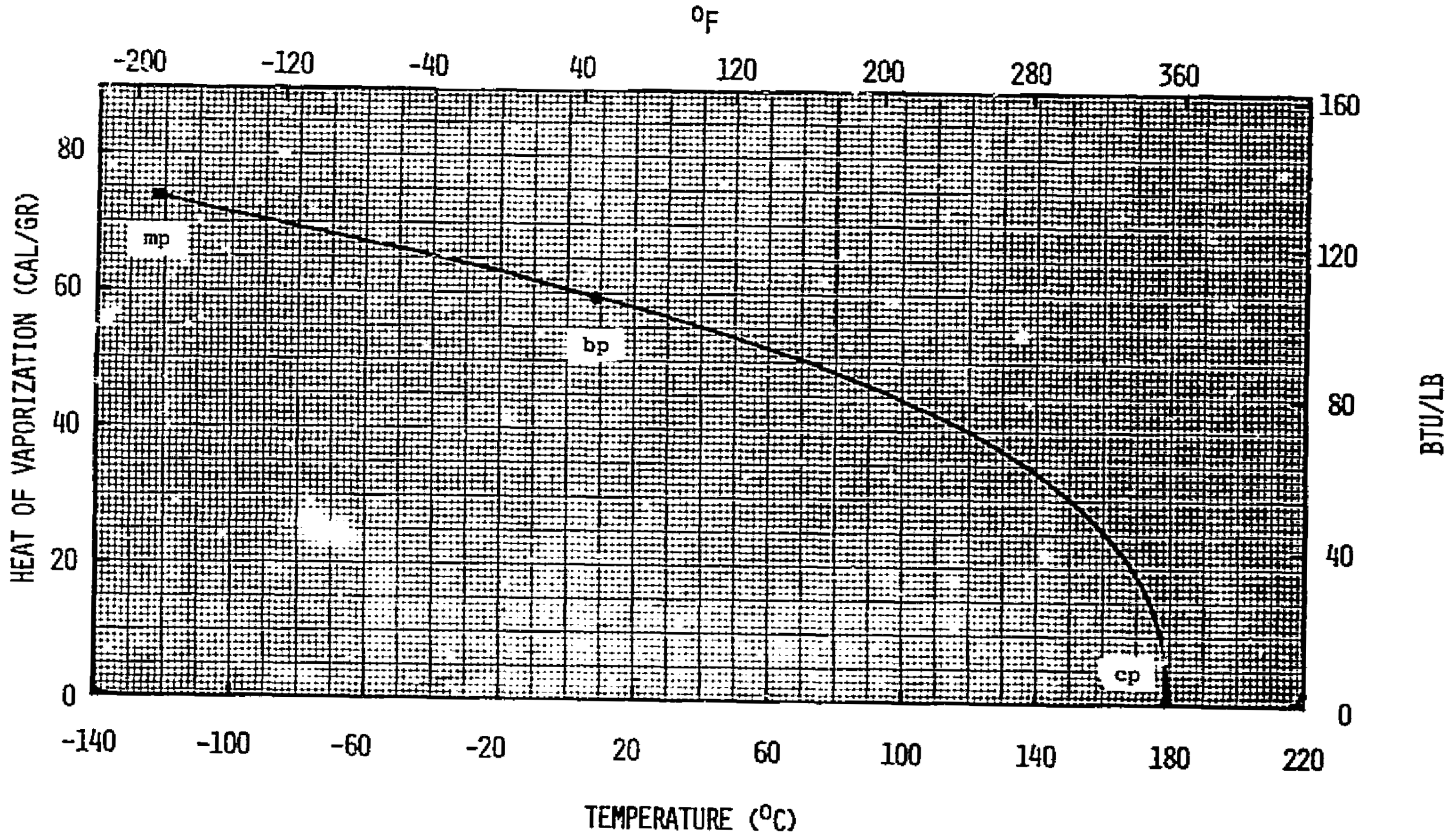

Figure 2.4-2 Heat of Vaporization vs Temperature for Dichlorosilane

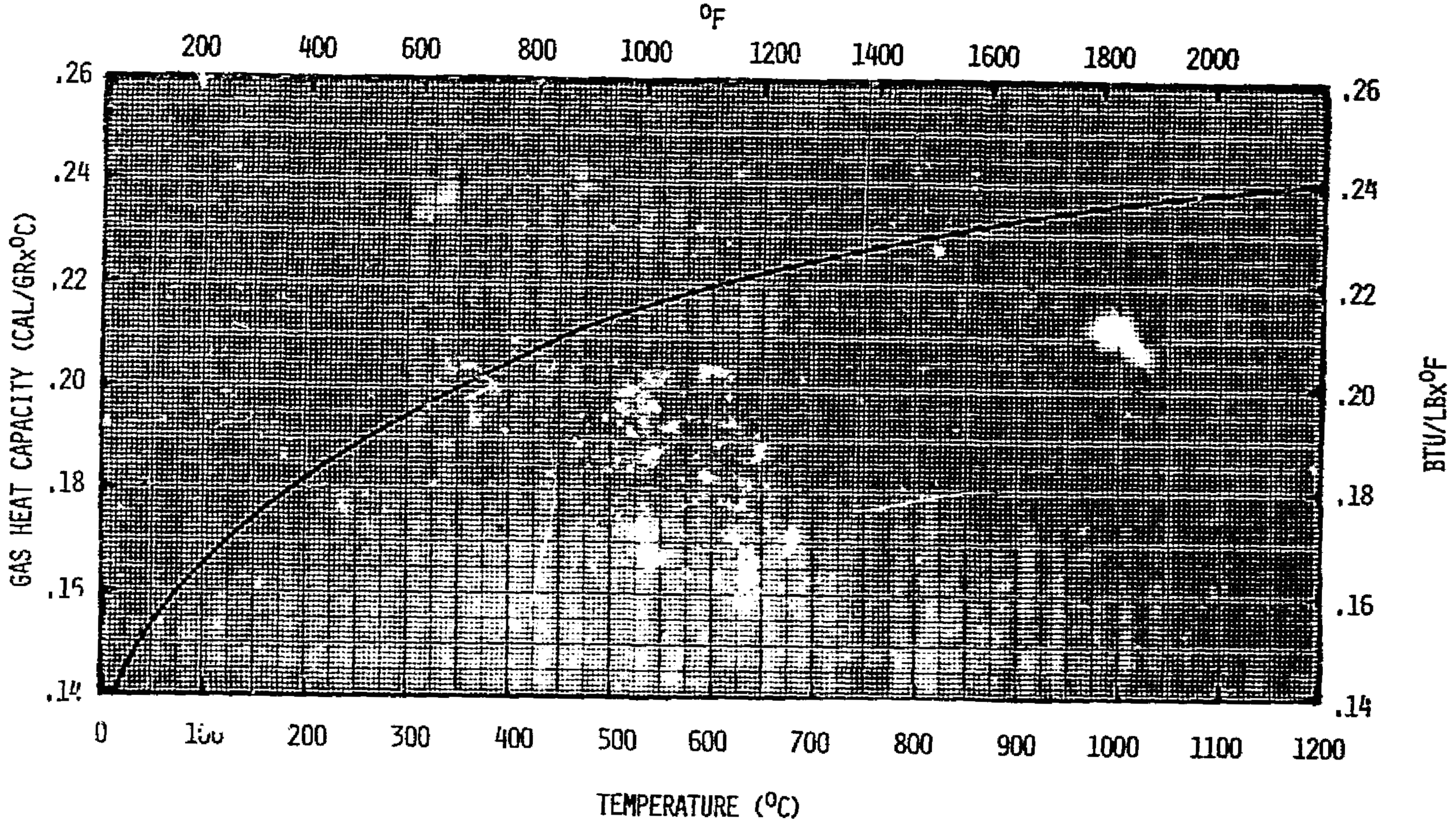

Figure 2.4-3 Gas Heat Capacity vs Temperature for Dichlorosilane

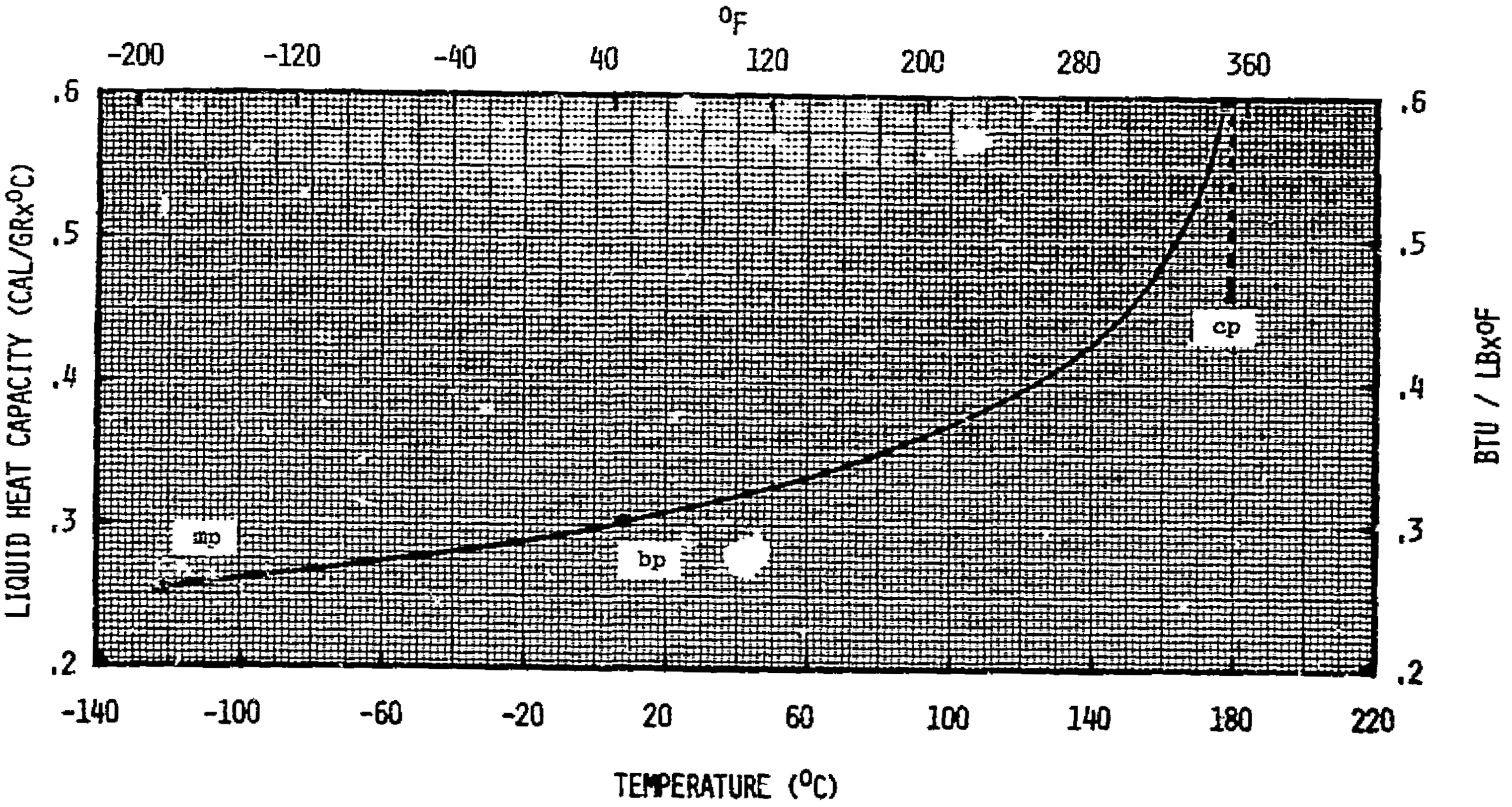

Figure 2.4-4 Liquid Heat Capacity vs Temperature for Dichlorosilane

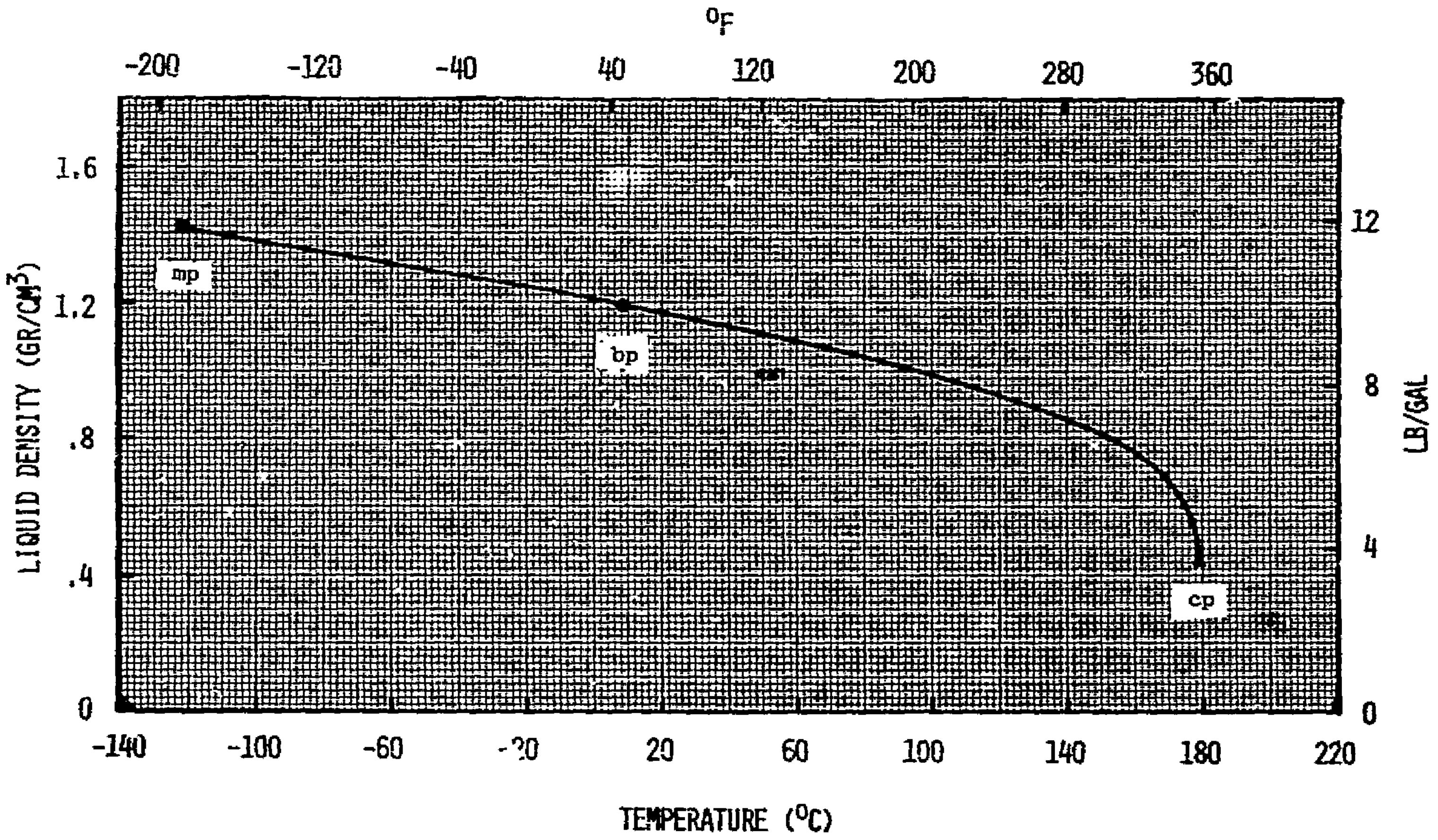

Figure 2.4-5 Liquid Density vs Temperature for Dichlorosilane

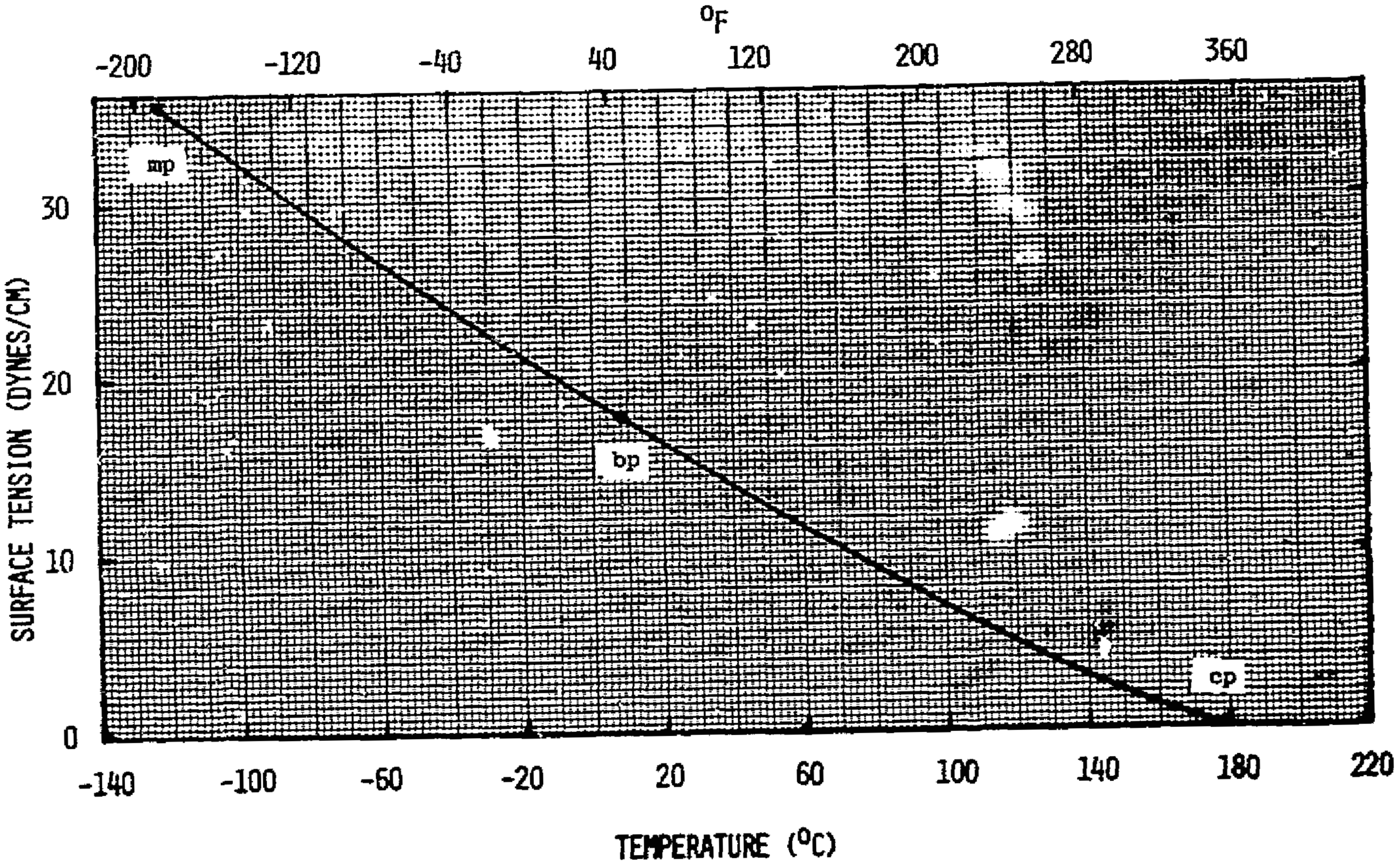

Figure 2.4-6 Surface Tension vs Temperature for Dichlorosilane

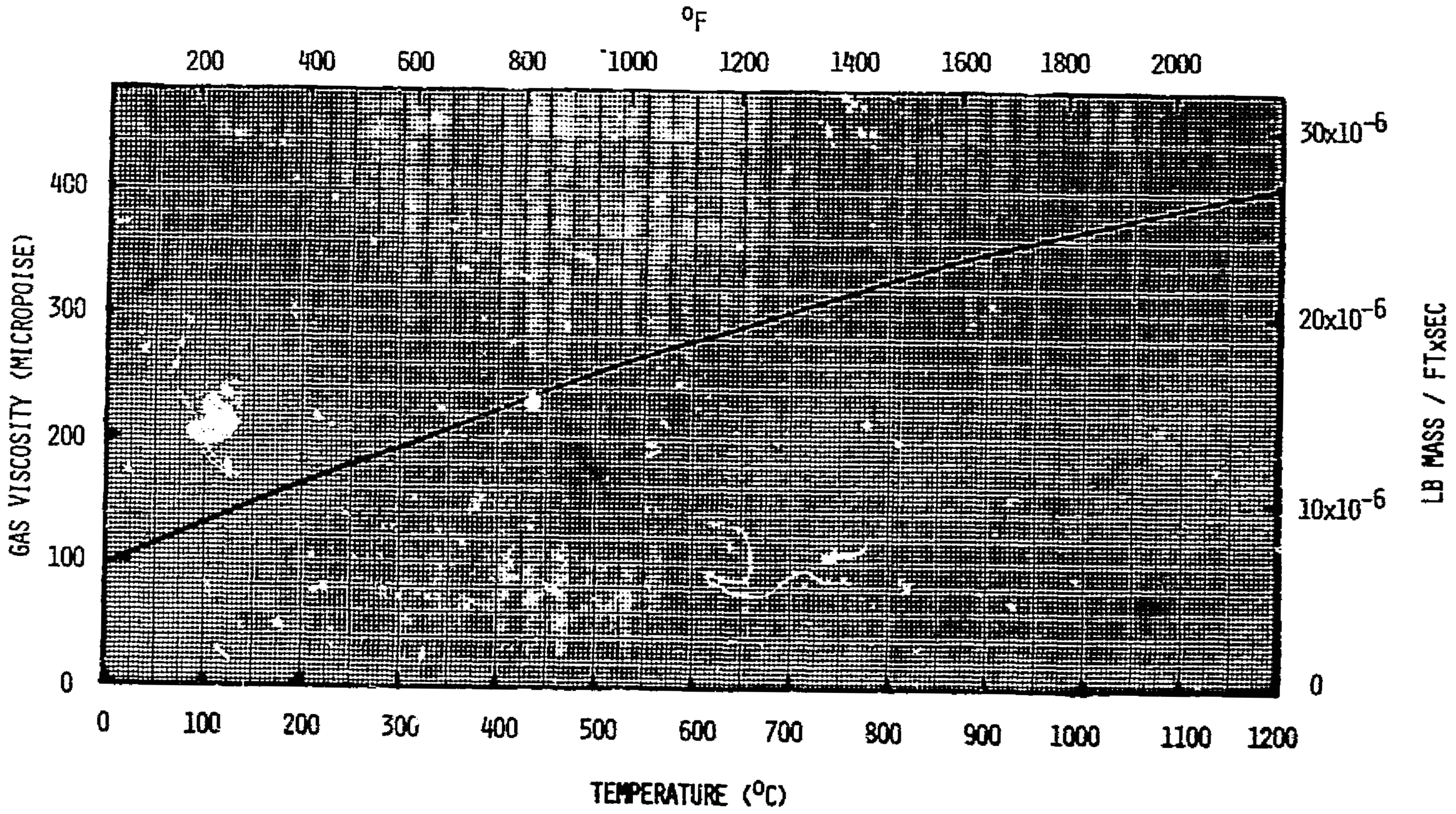

Figure 2.4-7 Gas Viscosity vs Temperature for Dichlorosilane

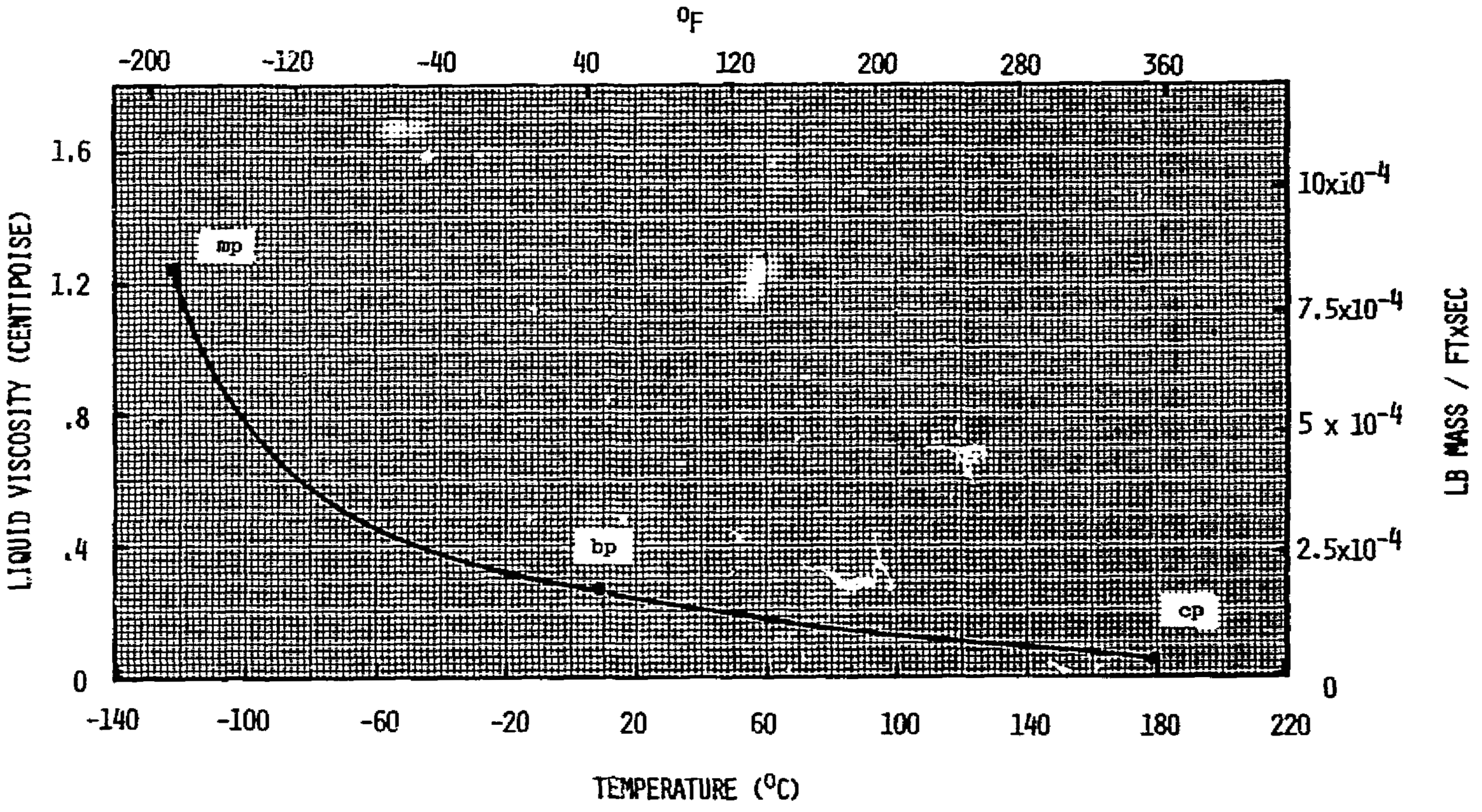

Figure 2.4-8 Liquid Viscosity vs Temperature for Dichlorosilane

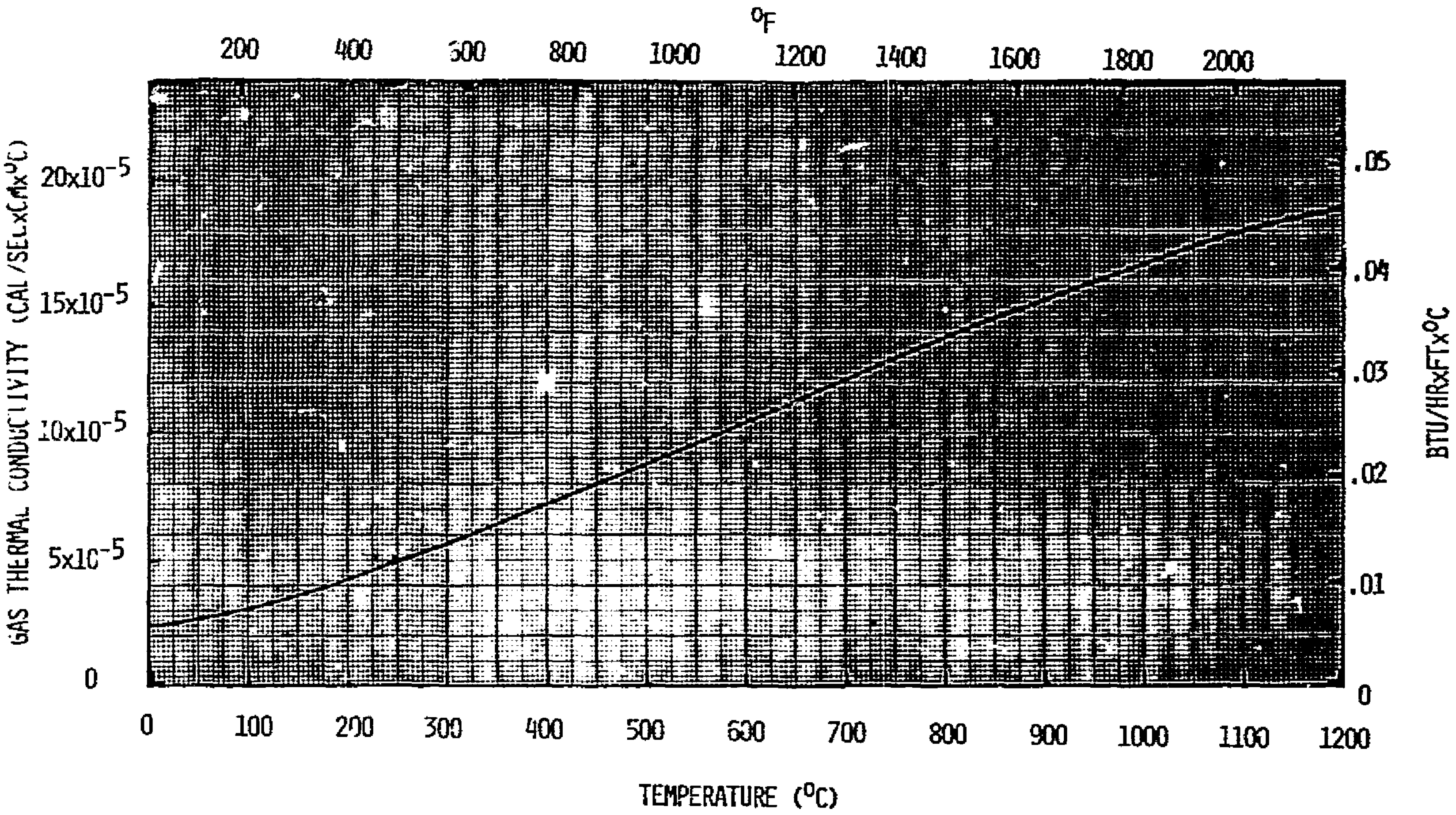

Figure 2.4-9 Gas Thermal Conductivity vs Temperature for Dichlorosilane

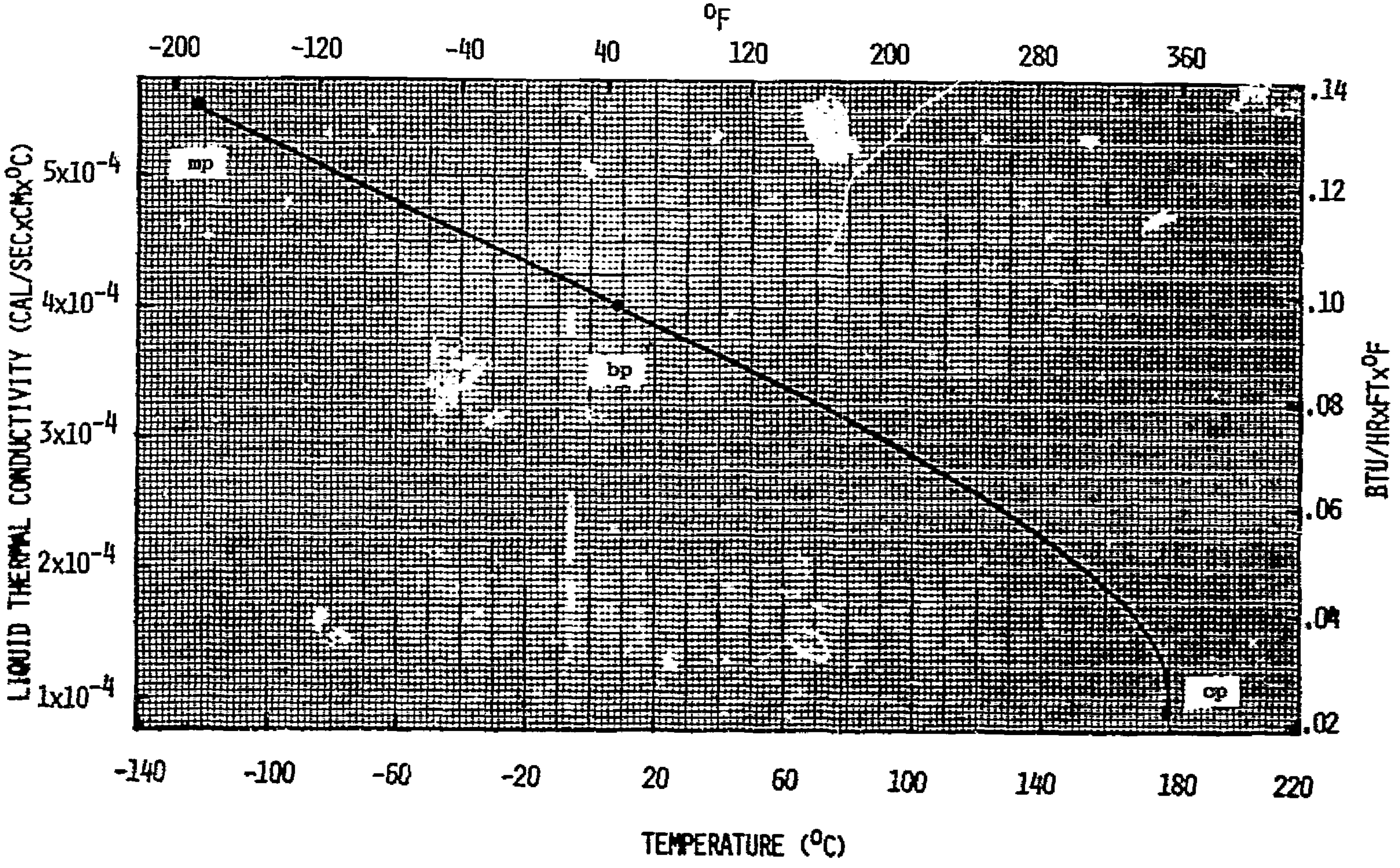

Figure 2.4-10 Liquid Thermal Conductivity vs Temperature for Dichlorosilane

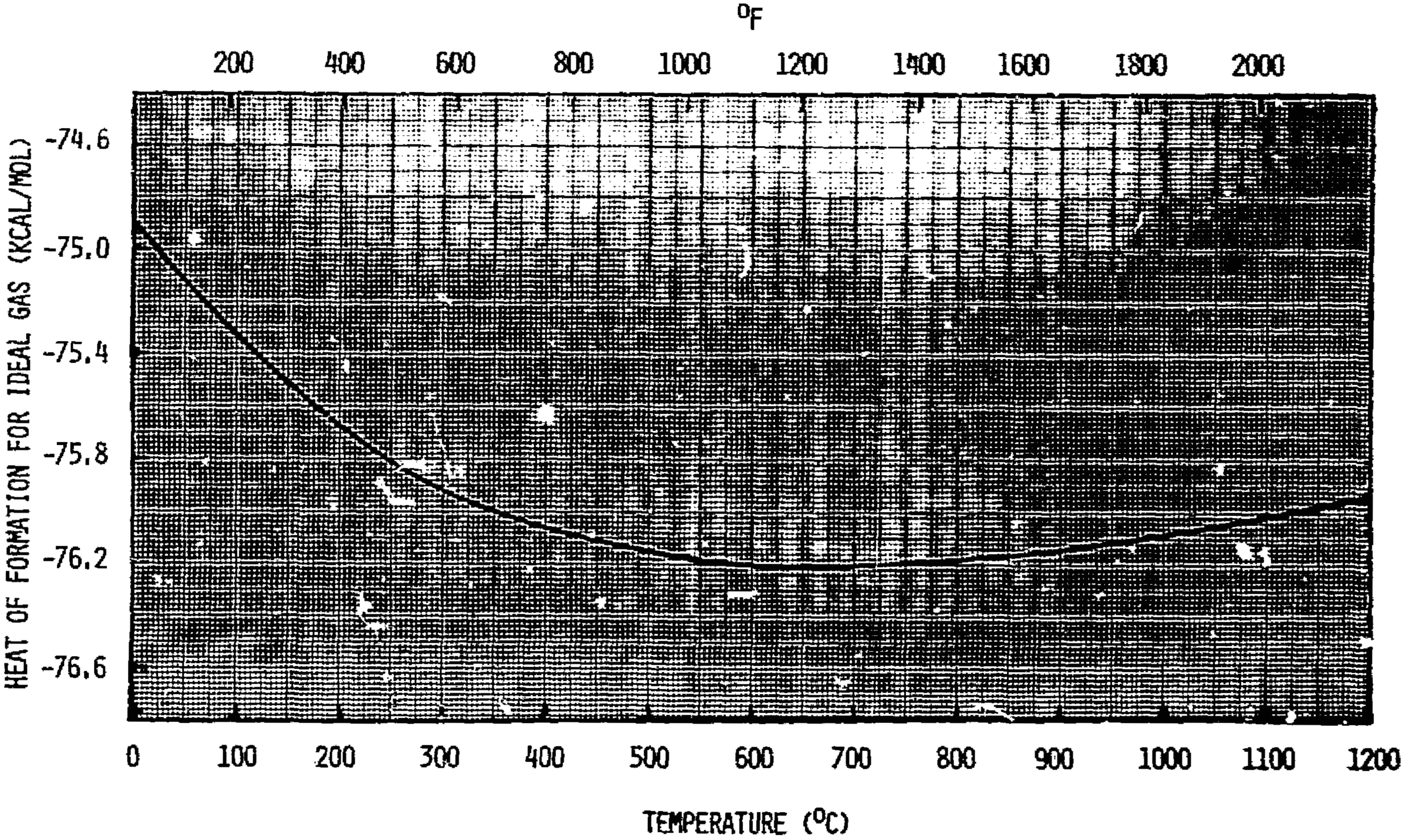

Figure 2.4-11 Heat of Formation vs Temperature for Dichlorosilane

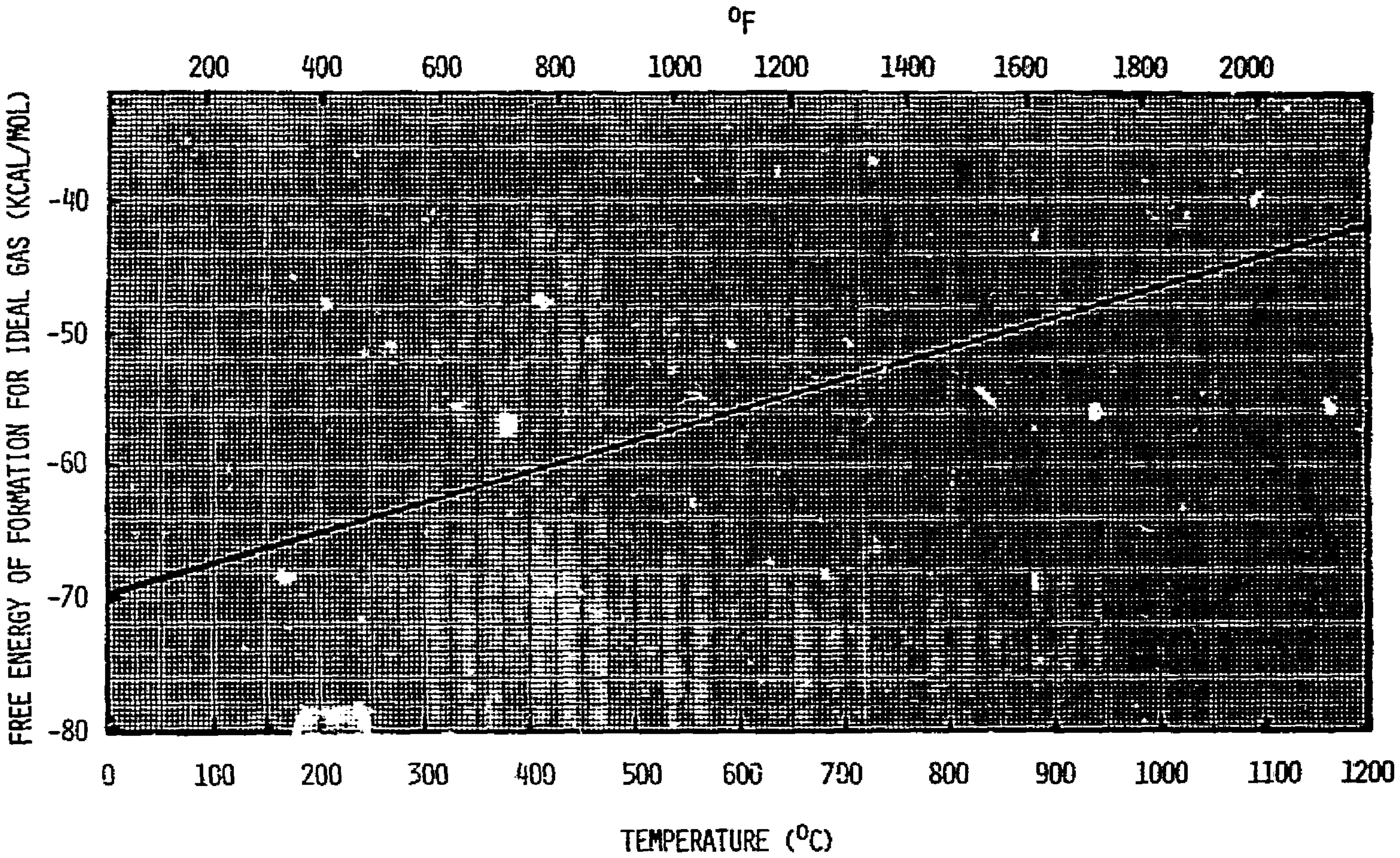

Figure 2.4-12 Free Energy of Formation vs Temperature for Dichlorosilane

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2.5 Silicon Tetrafluoride Properties

Physical Properties and Critical Constants (Table 2.5-1)

Physical properties are listed in Table IA-1 including the boiling point (sublimation temperature, where the vapor pressure of the solid is 760 mm Hg.). Two temperature are given in the literature for the melting point (triple point) of silicon tetrafluoride based on the work of Patnode and Papish (F37) in 1930 and the work of Pace and Mosser (F36) in 1963. The more recent work was selected as the melting point (triple point, where solid, liquid and vapor are in equilibrium).

Experimental data for the critical temperature and critical pressure of silicon tetrafluoride have been determined (F4). The critical compressibility factor, Z_c, was estimated from the Garcia'-Barcena' correlation (F39):

$$Z_c = f(T_b) - g(T_b/M) \qquad (2.5\text{-}1)$$

where T_b is the normal boiling point, °K, and M is the molecular weight. When this method was applied to sulfur hexafluoride, another subliming inorganic fluoride, the calculated value of the critical compressibility factor only deviated 3.3% from the known value. From the estimated value of Z_c, the critical volume, V_c, was calculated by the rearrangement of the definition of Z_c.

$$V_c = \frac{Z_c R T_c}{P_c} \qquad (2.5\text{-}2)$$

Vapor Pressure (Figure 2.5-1)

The vapor pressure of silicon tetrafluoride has been determined experimentally from 50° below the sublimation point to near the critical point (F4, F36, F37, F41). The experimental data were extended to cover the liquid range (from triple point to critical point), and for the solid (below the triple point using the YSSP correlation in each case:

$$\log P_v = A + \frac{B}{T} + C\log T + DT \qquad (2.5\text{-}3)$$

At the higher temperatures the deviation of experimental and correlation results are 2% while the average percent error was 4.8% in the lower temperature range. Much of the deviation is due to rather poor agreement in the literature for the experimenal values.

Heat of Vaporization (Figure 2.5-2)

Heat of vaporization data for silicon tetrafluoride are reported near the triple point (F24, F29, F36, F41, F60). Using the selected value (F36), Watson's correlation (F39) was used to extend the heat of vaporization over the entire liquid phase:

$$\Delta H_v = \Delta H_{v_1} \left[\frac{T_c - T}{T_c - T_1}\right]^n \qquad (2.5\text{-}4)$$

where $n = .38$ and T_1 is the boiling point. The value of H_{v_1} was effectively confirmed using the Clausius-Clapyron equation and literature vapor pressure values(F36).

Heat Capacity (Figures 2.5-3 and 2.5-4)

Heat capacity of the ideal gas at low pressure has been calculated from 0°C to 1200°C (F48, F63). These values, including other values covering smaller temperature ranges (F11, F24, F26, F29, F35, F60), were taken from various structural and spectral data and are in close argeement. The JANAF values (F48) were selected.

The liquid heat capacity of silicon tetrafluoride is reported near the sublimation point (F36). The values are extended over all liquid temperatures by the relationship:

$$\text{Heat Capacity} \times \text{Density} = \text{Constant} \qquad (2.5\text{-}5)$$

The estimated constant was 0.473. Testing of this relationship with available data (4 data points) for silicon tetrafluoride produced an average absolute deviation of 0.8% error.

Liquid Density (Figure 2.5-6)

Liquid density data for silicon tetrafluoride are available only within about 20 degrees of the triple point (F26, F60). The experimental data were extrapolated to the critical point by use of a modification of the Rackett equation (F65, F66):

$$\rho = \rho_c Z^{-(1-T_r)^{2/7}} \qquad (2.5\text{-}6)$$

where ρ_c is the critical density, T_r is the reduced temperature, and Z is a parameter derived from available data. Comparison of the calculated and experimental values of 5 data points gave 0.57% average absolute error.

Surface Tension (Figure 2.5-6)

Experimental data are not available for the surface tension of silicon tetrafluoride. The Brock and Bird corresponding states technique was used to estimate the surface tension (F39):

$$\alpha = P_c^{2/3} T_c^{1/3} (0.133\ \alpha_c - 0.281)(1-T_r)^{11/9} \qquad (2.5\text{-}7)$$

where α is surface tension, dynes/cm; α_c is the Riedel parameter; P_c is critical pressure, atm; T_c is the critical temperature, °K; and T_r is the reduced temperature. Application of this technique to silicon tetrachloride and sulfur hexafluoride gave results within 4% and 1% absolute deviation with experimental data, respectively.

Viscosity (Figures 2.5-7 and 2.5-8)

Experimental data for the gas viscosity of silicon tetrafluoride are available from about room temperature to above 300°C (F13, F32). The values at higher temperaures were estimated using the relationship:

$$\log \eta_G = A + BT + CT^2 \qquad (2.5\text{-}8)$$

The average absolute percentage error was 1.74% when correlated values were compared with the 28 experimental data points.

No experimental data are available for the liquid viscosity of silicon tetrafluoride. Estimates were derived applying the Letsou-Stiel high-temperature liquid-viscosity correlation (F65):

$$\eta_L\, \xi = (\eta_L \xi)^0 + \omega(\eta_L \xi)^1 \qquad (2.5\text{-}9)$$

where the parameters $(\eta_L \xi)^0$ and $(\eta_L \xi)^1$ are functions of reduced temperature, ω is the acentric factor and $\xi = T_c^{1/6}/M^{1/2}P_c^{2/3}$. This correlations gave results within 17% and 48% absolute deviaiton for the experimental values of silicon tetracloride and sulfur hexafluoride, respectively. Since liquid viscosity estimation methods may be grossly inaccurate (F69), these values must be assumed to be order of magnitude estimates only.

Thermal Conductivity (Figures 2.5-9 and 2.5-10)

The gaseous thermal conductivity of silicon tetrafluoride has been reported from about room temperature to 350°C (F9, F68). The experimental values were extended using a modified form of the Misic and Thodos correlation (F66):

$$\lambda_G = \frac{C_p}{\Gamma} (10^{-6}) (14.52 T_r - 5.14)^n \qquad (2.5\text{-}10)$$

where $n = .63$, Γ is $T_c^{1/6} M^{1/2} / P_c^{2/3}$, T_r is the reduced temperature and C_p is the gaseous heat capacity. The average percentage error was less than one percent.

No liquid thermal conductivity data are available; however, values were estimated using the Sato-Riedel equation (65):

$$\lambda_L = \frac{2.64 \times 10^{-3}}{M^{1/2}} \quad \frac{3 + 20(1-T_r)^{2/3}}{3 + 20(1-T_{r_b})^{2/3}} \qquad (2.5\text{-}11)$$

where M is molecular weight, T_r is the reduced temperature, and T_{r_b} is the reduced temperature at the boiling point. This correlation gave 34% error with the single experimental data point for silicon tetrachloride and 24% error for sulfur hexafluoride with the several experimental data points. There is considerable deviation of values among the several different data sources (22% maximum deviation). The present results should be taken only to represent an order of magnitude estimate.

Heat and Free Energy of Formation (Figures 2.5-11 and 2.5-12)

Many American workers (F20, F24, F29, F34, F35, F48, F57, F58) and others (F40, F43) have reported heats of formation was well as Gibb's free energy of formation (F48, F56, F58) for the ideal gas. The JANAF values (F48) were selected.

TABLE 2.5-1

PHYSICAL PROPERTIES AND CRITICAL CONSTANTS OF SILICON TETRAFLUORIDE

Identification	Silicon Tetrafluoride
Formula	SiF_4
State (std. cond.)	gas (colorless)
Molecular weight, M	104.08
Boiling point, T_b, °C (sublimation point)	-95.7 (760 mm Hg)
Melting Point, T_m, °C (triple point)	-86.8 (1679 mm Hg)*Ref. F36 -90.2 (1318 mm Hg) Ref. F37
Critical Temp, T_c, °C	-14.15
Critical Pressure, P_c, atm	36.66
Critical Volume, V_c, cm^3/gr mol	165**
Critical Compressibility Factor, Z_c	0.284**
Critical Density, ρ_c. gr/cm^3	0.6308**
Acentric Factor (ω)	0.4086

* Selected Value

**Estimated

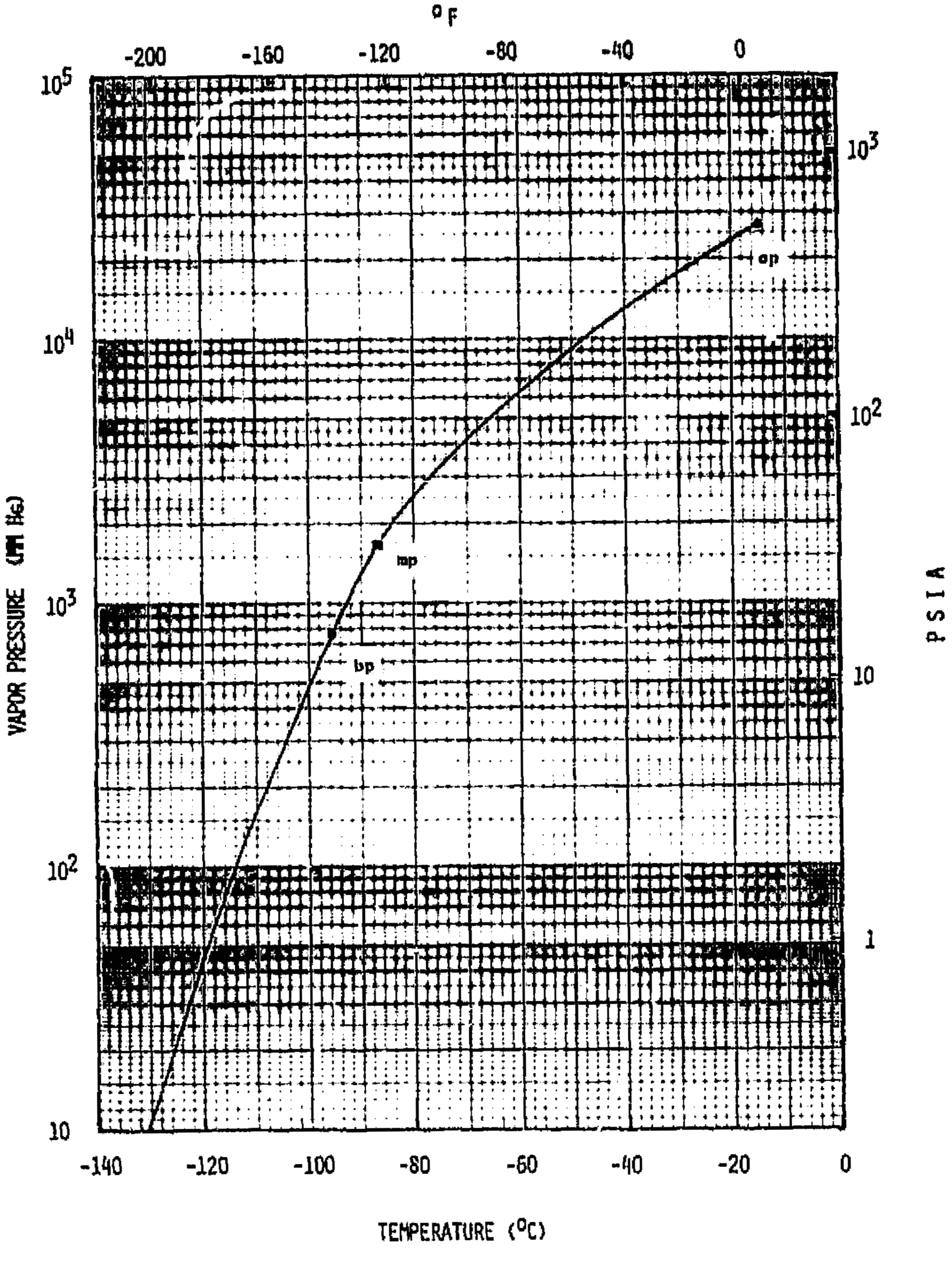

Figure 2.5-1 Vapor Pressure vs Temperature for Silicon Tetrafluoride

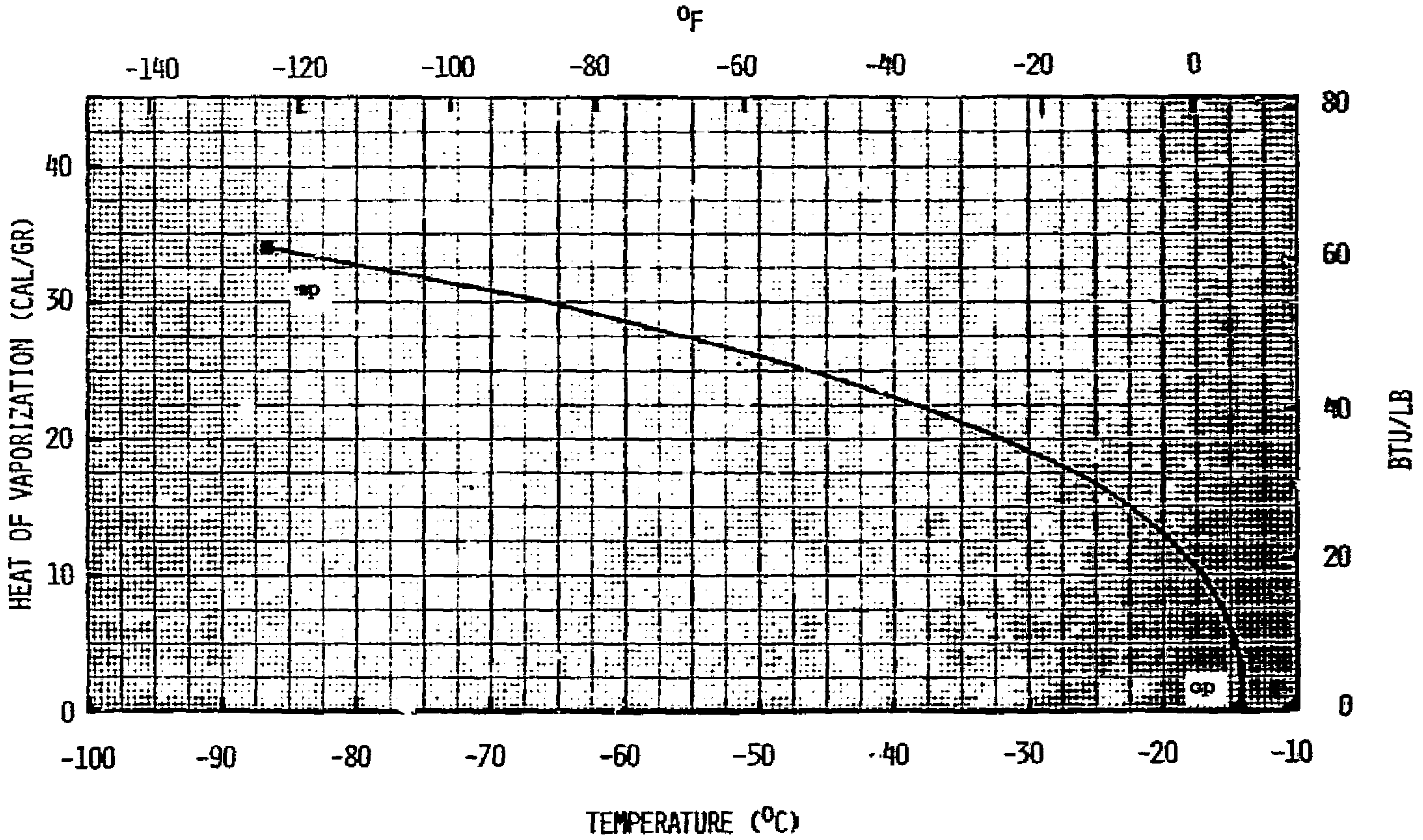

Figure 2.5-2 Heat of Vaporization vs Temperature for Silicon Tetrafluoride

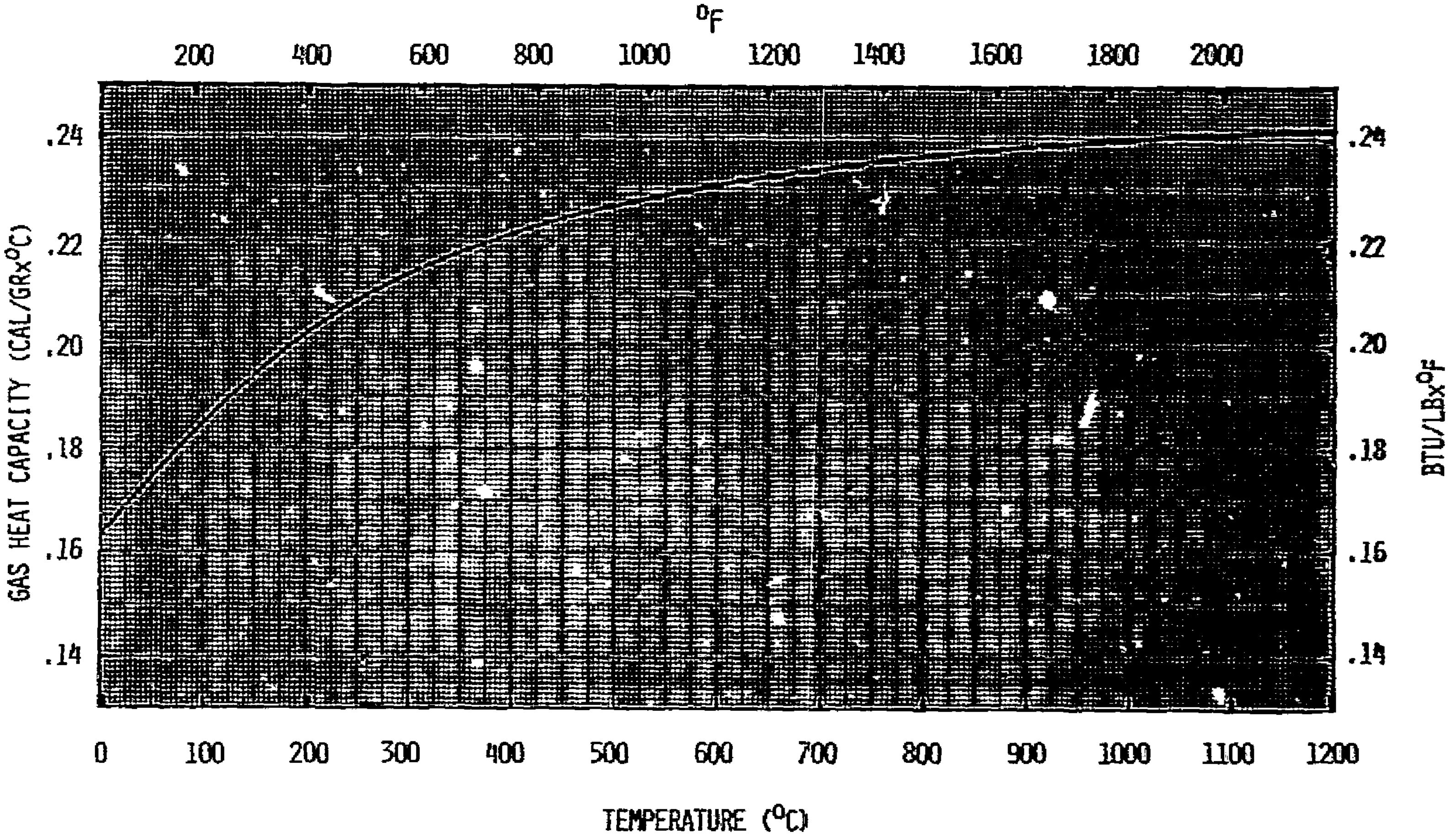

Figure 2.5-3 Gas Heat Capacity vs Temperature for Silicon Tetrafluoride

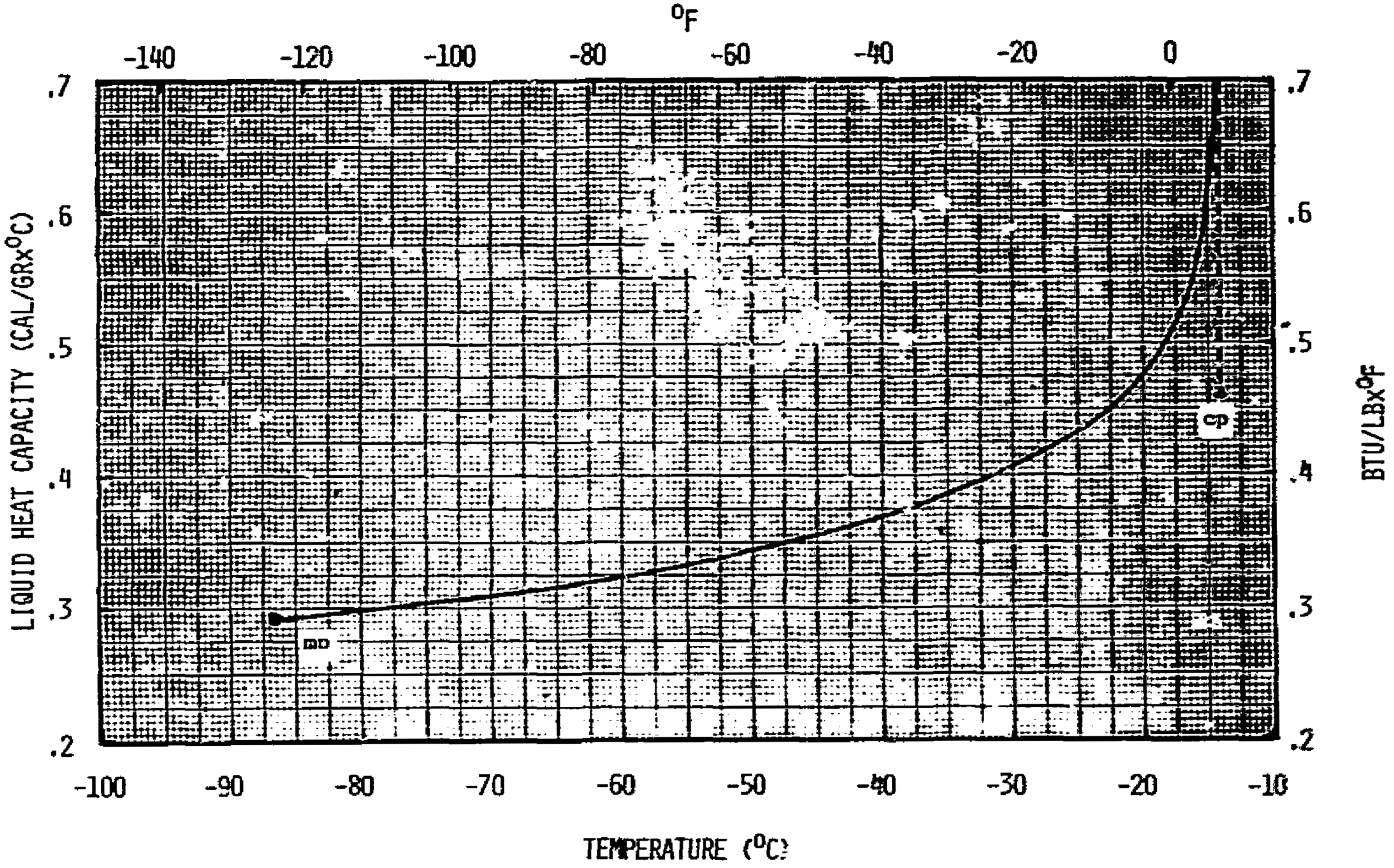

Figure 2.5-4 Liquid Heat Capacity vs Temperature for Silicon Tetrafluoride

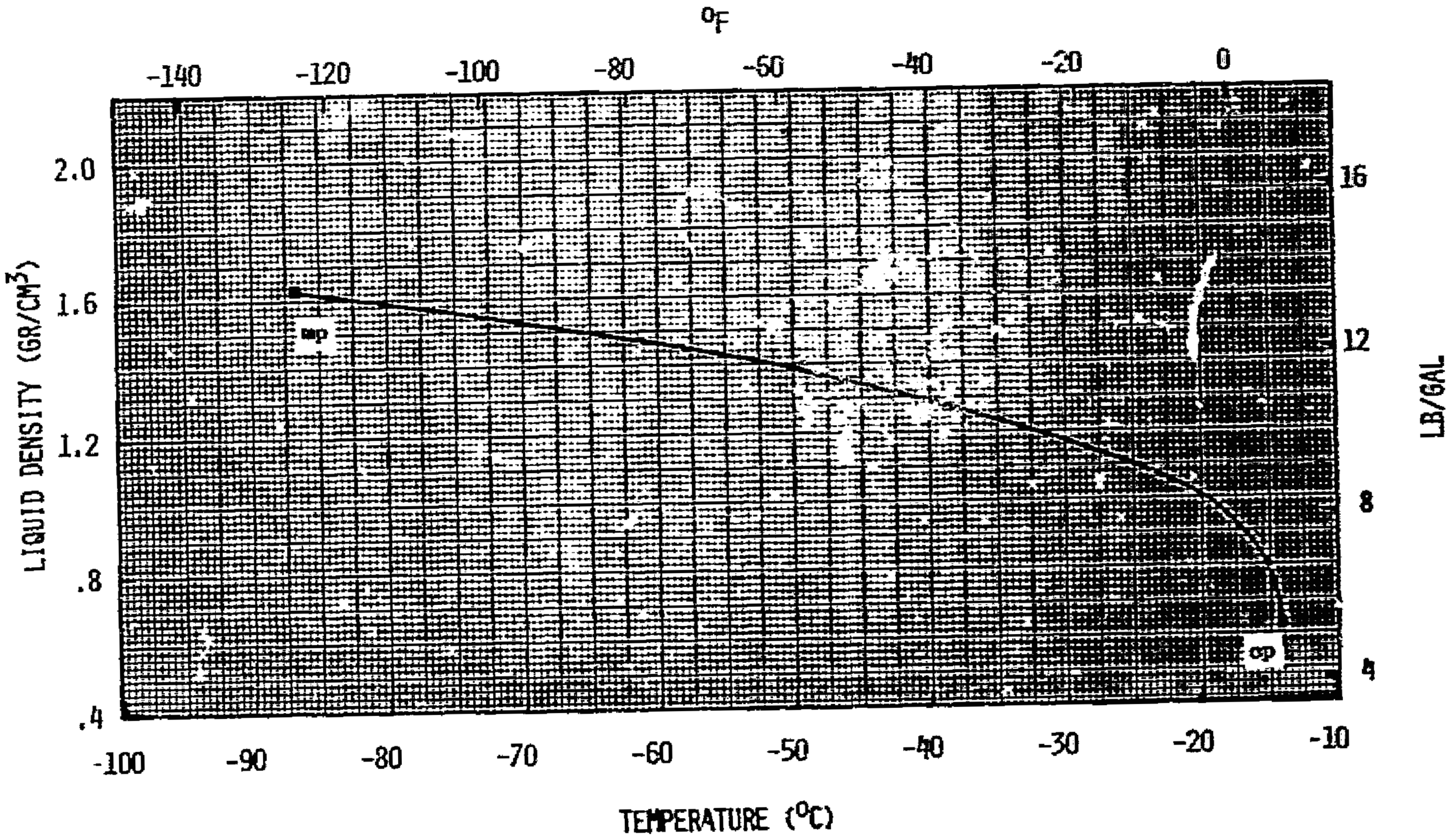

Figure 2.5-5 Liquid Density vs Temperature for Silicon Tetrafluoride

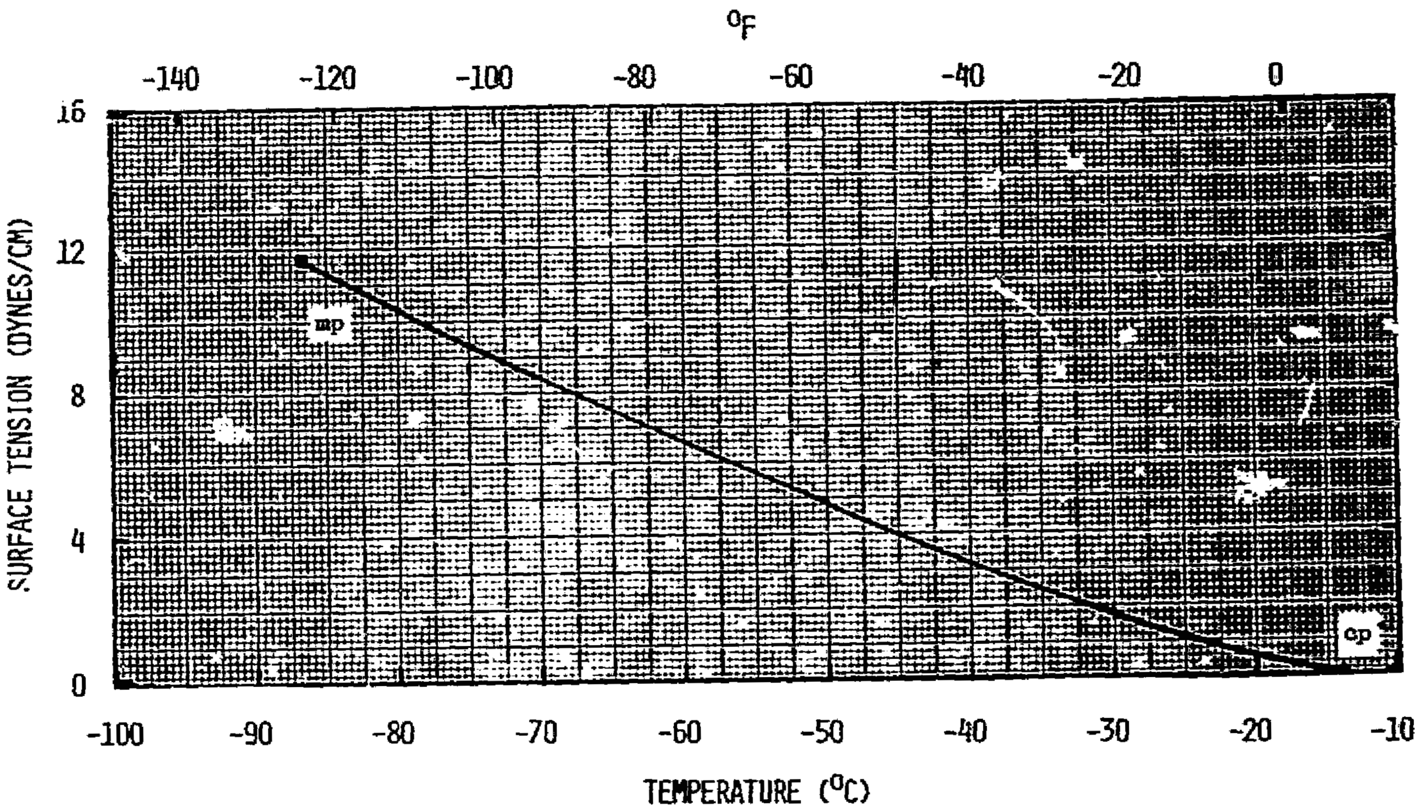

Figure 2.5-6 Surface Tension vs Temperature for Silicon Tetrafluoride

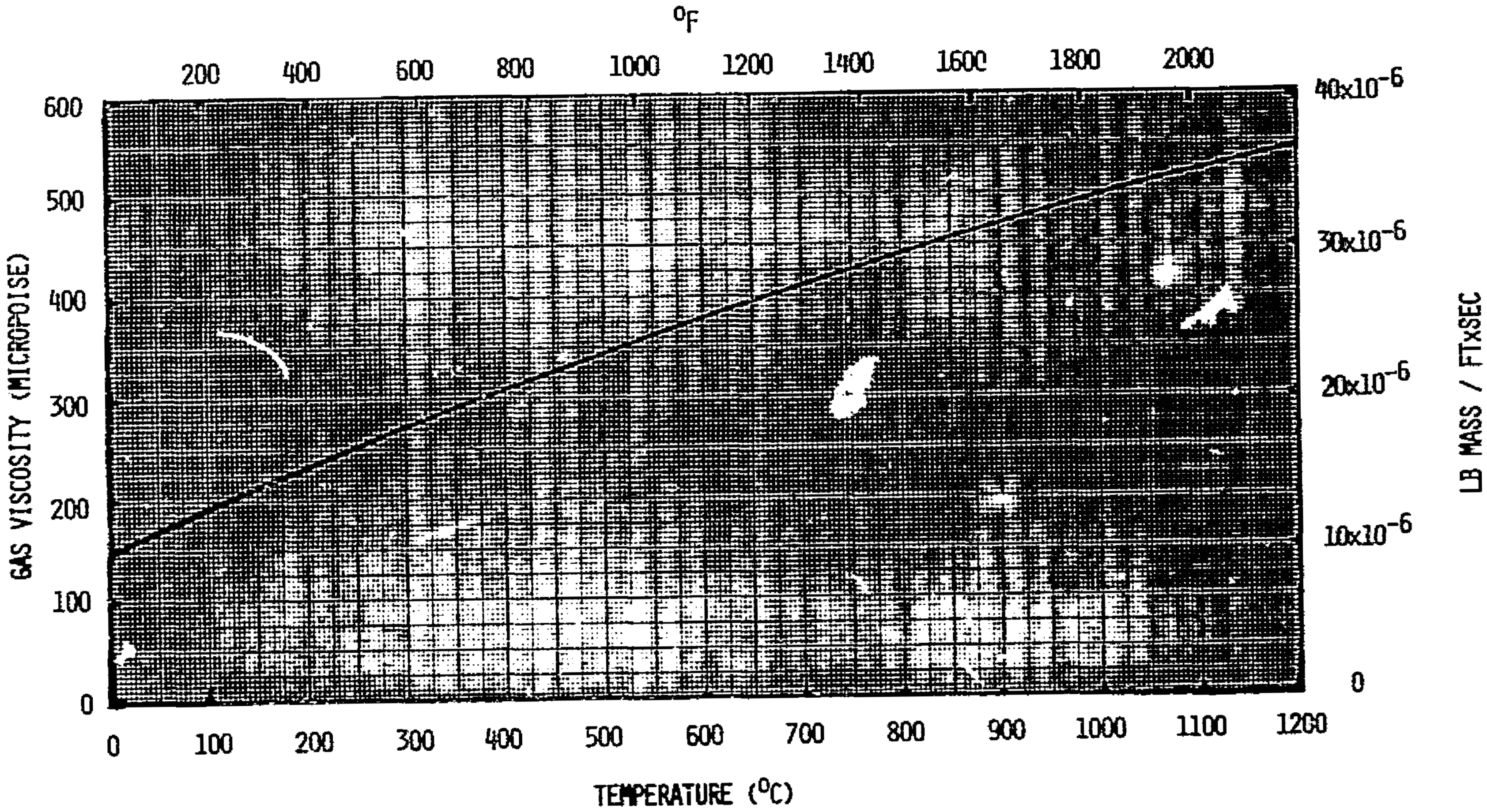

Figure 2.5-7 Gas Viscosity vs Temperature for Silicon Tetrafluoride

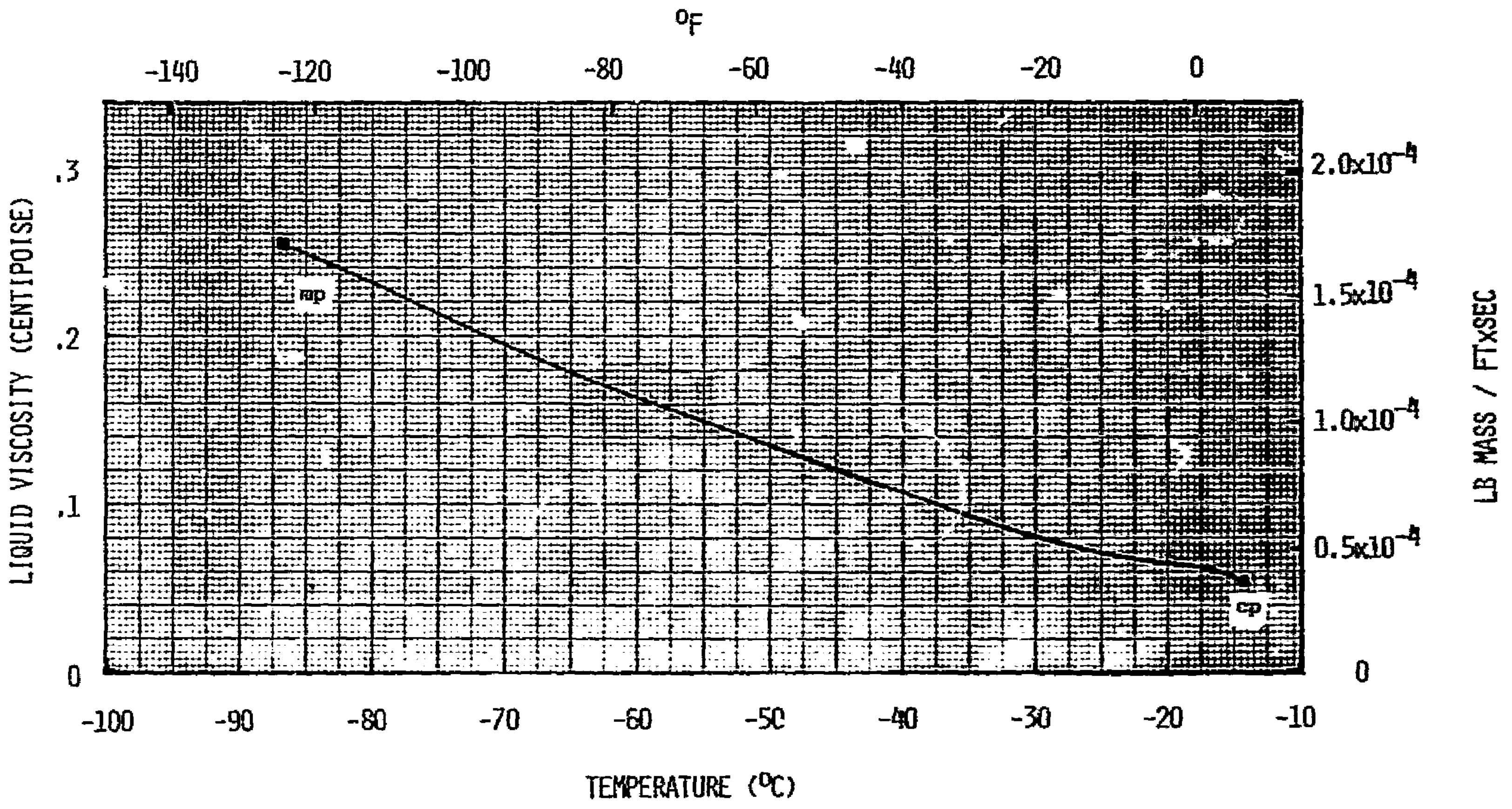

Figure 2.5-8 Liquid Viscosity vs Temperature for Silicon Tetrafluoride

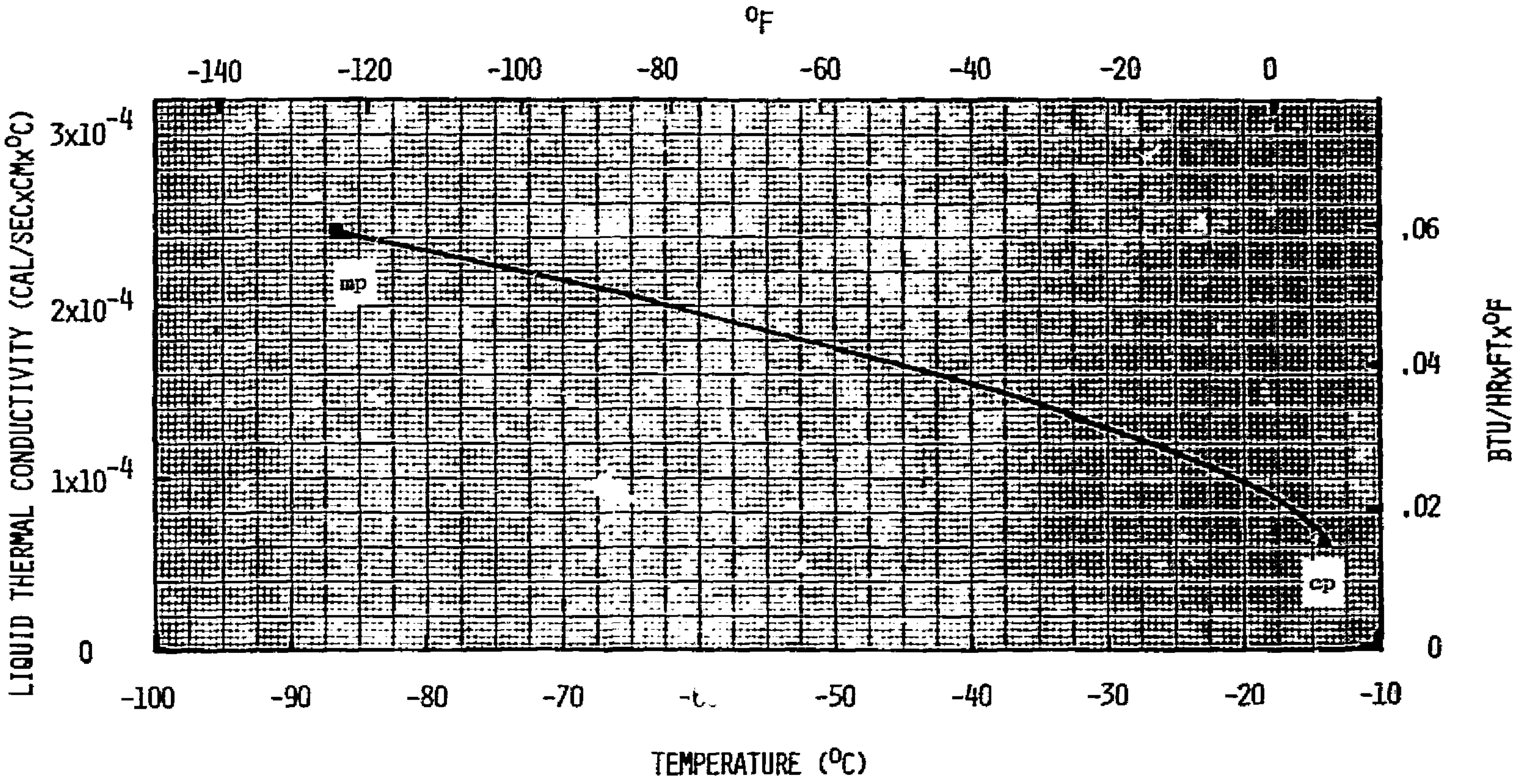

Figure 2.5-10 Liquid Thermal Conductivity vs Temperature for Silicon Tetrafluoride

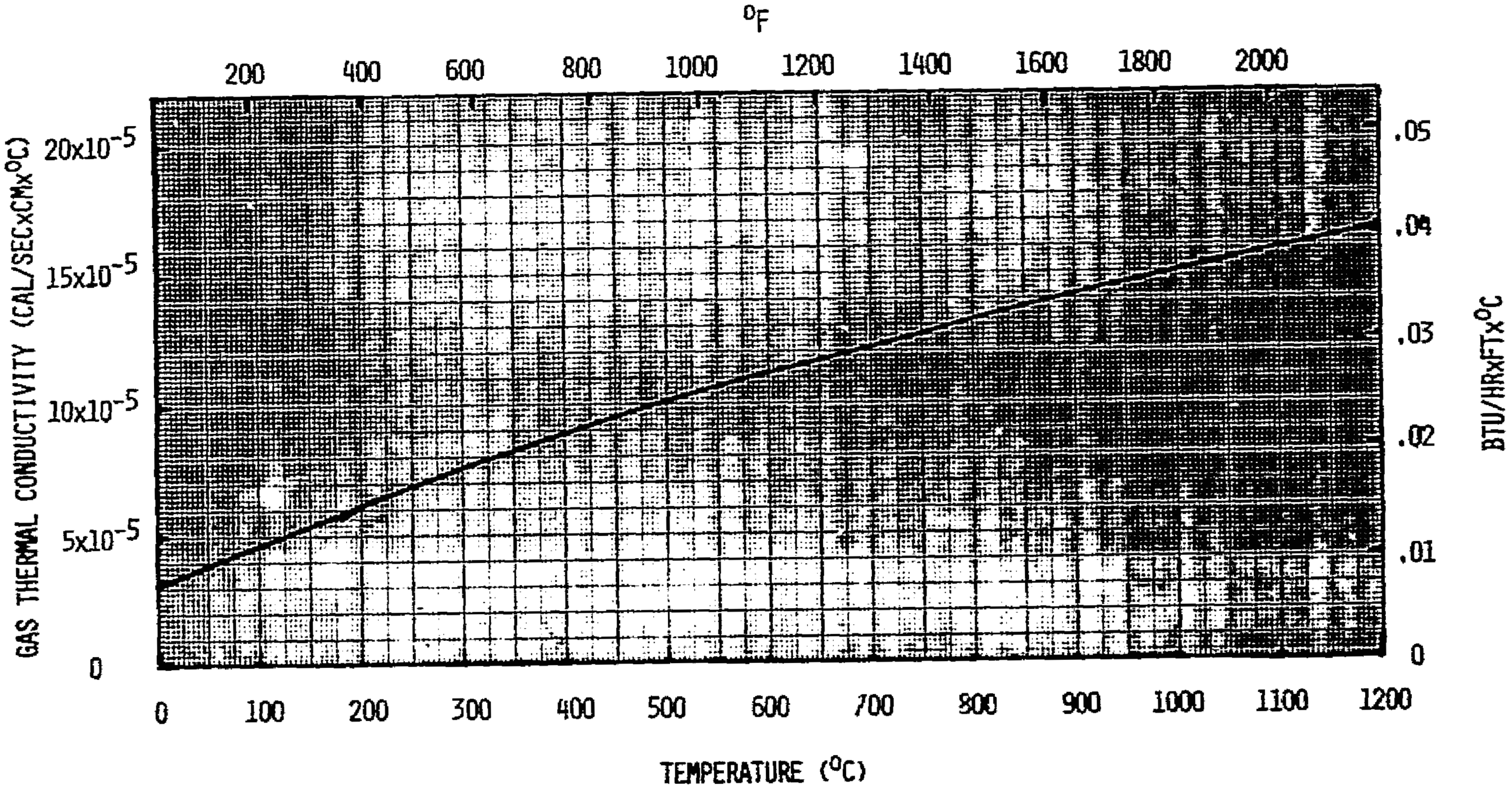

Figure 2.5-9 Gas Thermal Conductivity vs Temperature for Silicon Tetrafluoride

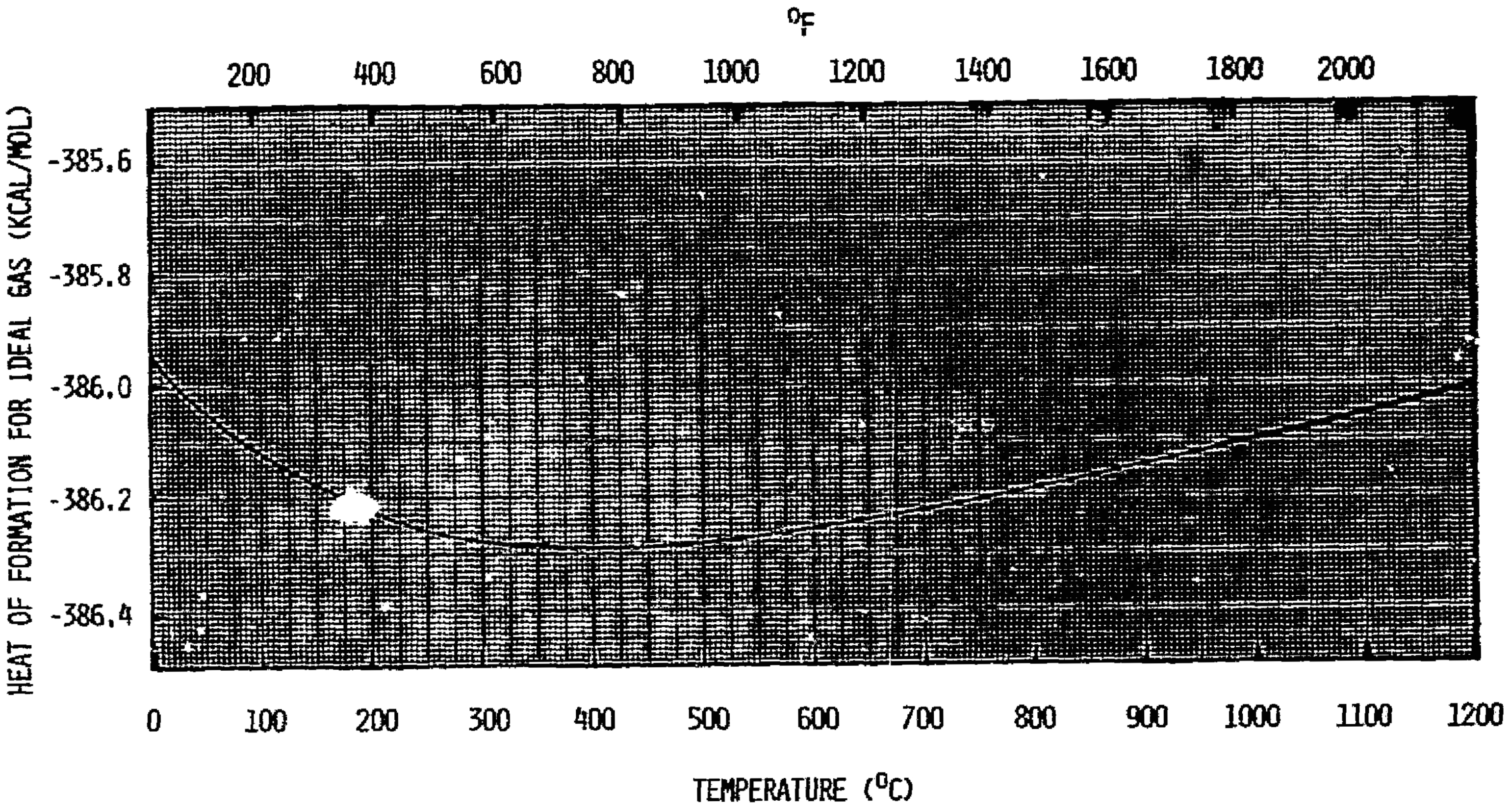

Figure 2.5-11 Heat of Formation vs Temperature for Silicon Tetrafluoride

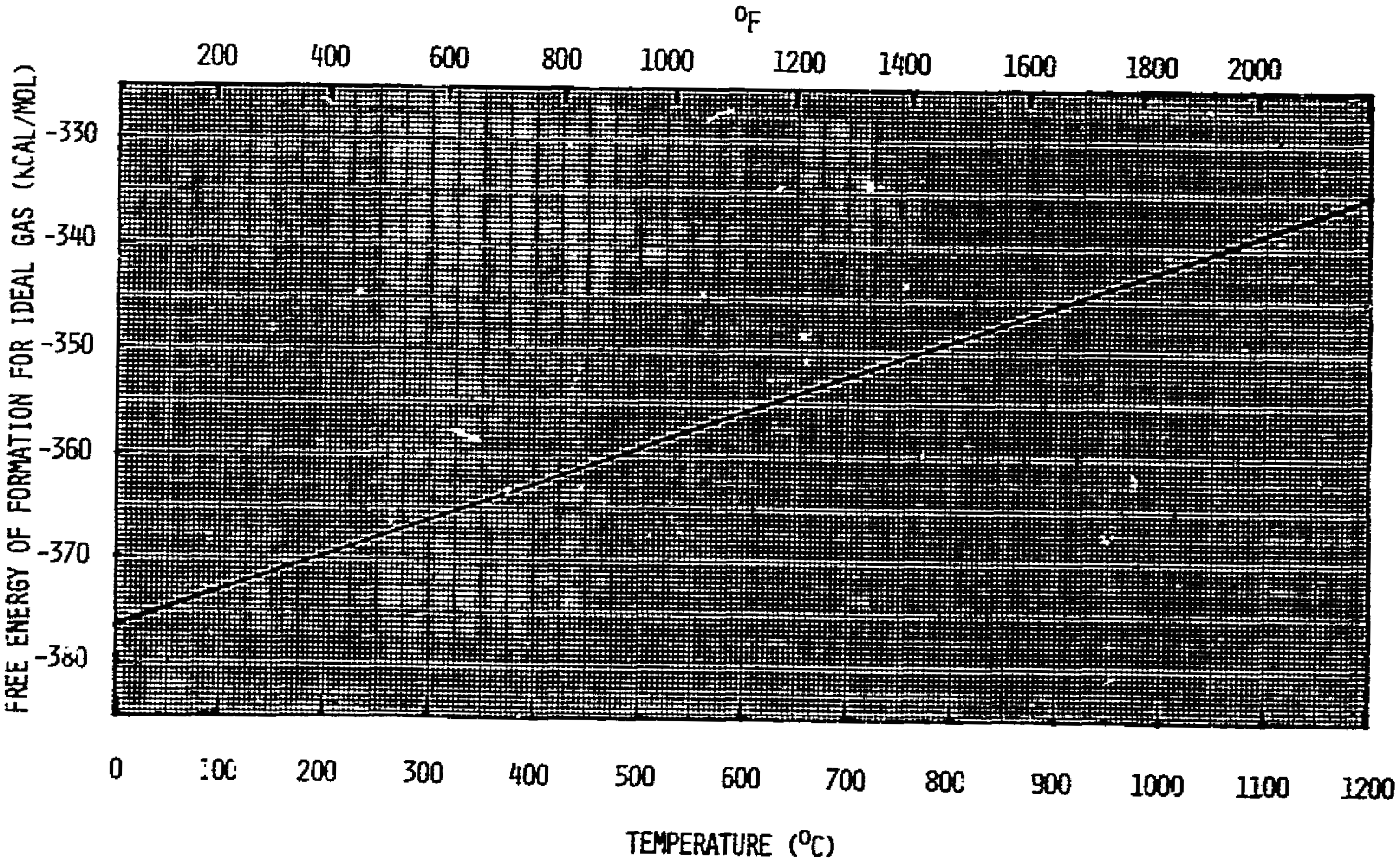

Figure 2.5-12 Free Energy of Formation vs Temperature for Silicon Tetrafluoride

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2.6 Silicon Properties

PHYSICAL PROPERTIES (TABLE 2.6-1)

Experimental values for the melting point have been reported (1, 32, 49, 67, 110); however, all other values have been calculated. Estimated values for the boiling point range from 2285°C to 3267°C (10, 31, 52, 55, 109, 124, 125, 137). Our value is estimated to give a reasonable computer fit to the available vapor pressure data. Estimated values of critical properties are reported by van Laar's calculation (5, 34, 43, 44, 101, 125), Baibus (4) and Gates and Thodos (31, reported in Table I-1). Solid properties listed in Table I-1 are at room temperature while liquid properties are at the melting point.

VAPOR PRESSURE (FIGURE 2.6-1)

Recent vapor pressure data reported by American (1, 18) and British (6) workers were selected and extended using the YSSP vapor pressure correlation (157):

$$\log P_V = A + \frac{B}{T} + C \log T + DT + ET^2 \qquad (2.6\text{-}1)$$

where P_V is the vapor pressure of saturated liquid, mm Hg; T is temperature, °K; and A, B, C, D and E are correlation constants derived using a generalized least squares program. Other data (10, 125, 142) were not used because of high percentage error which is reported to be due to extensive reaction of the silicon (54, 165). For the 44 experimental data points used (which are all in the range below 0.2 mm Hg) the average absolute deviation was 17%.

HEAT OF VAPORIZATION (FIGURE 2.6-2)

Heat of vaporization values of about 3850 cal/gm are available (1, 6, 18, 55) as well as older (10, 125a, 147) and Russian (142) values of about 3170 cal/gm. From the vapor pressure data near the melting point, the heat of vaporization was determined using the Clausius-Clapyrin equation. Using these values, Watson's correlation (165) was used to extend the heat of vaporization to the boiling point.

$$\Delta H_V = \Delta H_{V_1} \left[\frac{7500 - T}{7500 - T_1} \right]^n \qquad (2.6\text{-}2)$$

where $n = 0.38$ and all other terms have their usual meanings. The calculated values give a 1.3% absolute percentage deviation with the five experimental references giving values near 3850 cal/gm near the melting point.

HEAT OF SUBLIMATION (FIGURE 2.6-3)

Heat of sublimation based on limited data have been reported recently in the literature (18, 54, 106). Using the YSSP correlation of vapor pressure data (as described earlier), heats of sublimation were calculated using the Clausius-Clapeyron equation (123):

$$\Delta H_{sub} = P \Delta V_{sub} \frac{\delta P}{\delta T} \qquad (2.6\text{-}3)$$

where ΔH_{sub} is the heat of sublimation, cal/gr-mol; P is the vapor pressure, atm; and $\Delta V_{sub} = V_{gas} - V_{solid}$. The derivative, $\delta P/\delta T$, was determined from differentiation of the YSSP vapor pressure equation. Considering the possible inaccuracy in the extrapolation of very low vapor pressures at low temperatures, these values should be considered only order-of-magnitude calculations below 600°C.

HEAT CAPACITY (FIGURES 2.6-4 and 2.6-5)

Liquid heat capacities have been reported from experiments done in the range from the melting point to about 200°C above the melting point (67, 100). The values of Kantur (67) were selected because the temperature range was significantly greater with the temperatures appearing to be more accurately determined. The average values of heat capacity and temperature were taken as a reference point and the values were extended over the liquid range using the relationship:

$$\text{Liquid Heat Capacity} \times \text{Liquid Density} = \text{constant} \qquad (2.6\text{-}4)$$

Calculated values agree within two percent of the values published in the experimental work (67).

Solid heat capacities have been reported by many authors (144, 138, 55, 34, 96, 164, 62, 115, and others) which give similar values. The JANAF and Touloukian values (138, 144) were selected.

DENSITY (FIGURES 2.6-6 & 2.6-7)

Several authors (93, 37, 14, 25, 9) have reported measured liquid density values from the melting point to about 400°C above the melting point. The datawere extended to the boiling point using a modification of the Rackett equation (166):

$$\rho = \rho_c \, z^{-(1 - T_r)^{2/7}} \qquad (2.6\text{-}5)$$

where ρ_c is critical density; T_r is reduced temperature and z is a parameter defined by the experimental data. Calculated values give a 0.5% average absolute deviation from the thirty reported experimental values. The vertical line at the melting point indicates the change in density upon melting.

Solid density measurements of silicon are recorded near room temperature (133, 134) at the melting point (85) and many others give linear thermal expansion data which are summarized by Touloukian (144). Solid densities at various temperatures were calculated using the percentage linear expansions (144) according to the relation:

$$\rho = \rho_1 \times \{1 - [3x(\text{percent linear expansion})]\} \qquad (2.6\text{-}6)$$

Calculated values gave less than one percent deviation with the measured values over the solid range.

SURFACE TENSION (FIGURE 2.6-8)

Limited data for the surface tension of silicon show a wide range of values (79, 71, 130, 25, 40). From the experimental data in close agreement (79, 71, 130), values were extended to the boiling point using the Othmer relation (123):

$$\sigma = \sigma_1 \left[\frac{7500 - T}{7500 - T_1} \right]^n \qquad (2.6\text{-}7)$$

where σ is surface tension at T_1, dynes/cm, and n is the correlation parameter, 1.2. The other parameters have their usual meaning. Calculated values agree with the limited data (5 values) with a 1.5% absolute error.

LIQUID VISCOSITY (FIGURE 2.6-9)

Liquid viscosity data for silicon are available from the melting point to about 400°C above the melting point (9, 81, 127, 163). Values from the melting point to the boiling point were calculated using a log η_L vs 1/T linear relationship. Average absolute percentage error was 9.1% on 19 data points, due largely to the wide scatter of the experimental data.

THERMAL CONDUCTIVITY (FIGURE 2.6-10)

An experimental value of the liquid thermal conductivity of silicon has been reported by Russian workers (167). Their research indicates a value of 0.16 (± .02) cal/cm × sec × °C at the melting point. The higher value of the thermal conductivity of liquid silicon compared to solid silicon at the melting point is in agreement with other experimental work (168).

Solid thermal conductivity data has been reported by several authors (104, 23, 83 and others). The recommended values of Touloukian (144) were selected.

TABLE 2.6-1

PHYSICAL PROPERTIES AND CRITICAL CONSTANTS OF SILICON

No.	Identification	Silicon
1.	Symbol	Si
2.	State (std. cond.)	Solid
3.	Atomic Weight	28.086
4.	Boiling Point, b.p., °C	2,878*
5.	Melting Point, m.p., °C	1,412 ± 2
6.	Critical Temperature, T_c, °C	4,886*
7.	Critical Pressure, P_c, atm	530*
8.	Critical Volume, V_c, cm^3/gr mol	232.6*
9.	Critical Density, ρ_c, gr/cm^3	0.1207*
10.	Vapor Pressure, mm Hg	2.8×10^{-4} (at m.p.)
11.	Heat of Vaporization, cal/gr	3,812 (at m.p.)
12.	Heat of Sublimation, cal/gr	4,075 (at m.p.)
13.	Heat of Fusion, cal/gr	264* (at m.p.)
14.	Liquid Heat Capacity, cal/gr-mol °C	6.755 (at m.p.)
15.	Solid Heat Capacity, cal/gr-mol °C	4.78 (at 25°C)
16.	Liquid Density, gr/cm^3	2.533 (at m.p.)
17.	Solid Density, gr/cm^3	2.329 (at 25°C)
18.	Percent Expansion on Freezing	10% (at m.p.)
19.	Surface Tension, dynes/cm	736 (at m.p.)
20.	Liquid Viscosity, centipoise	0.88 (at m.p.)
21.	Liquid Thermal Conductivity, cal/secxcmx°C	0.16 (at m.p.)
22.	Solid Thermal Conductivity, cal/secxcmx°C	0.353 (at 25°C)

*estimated

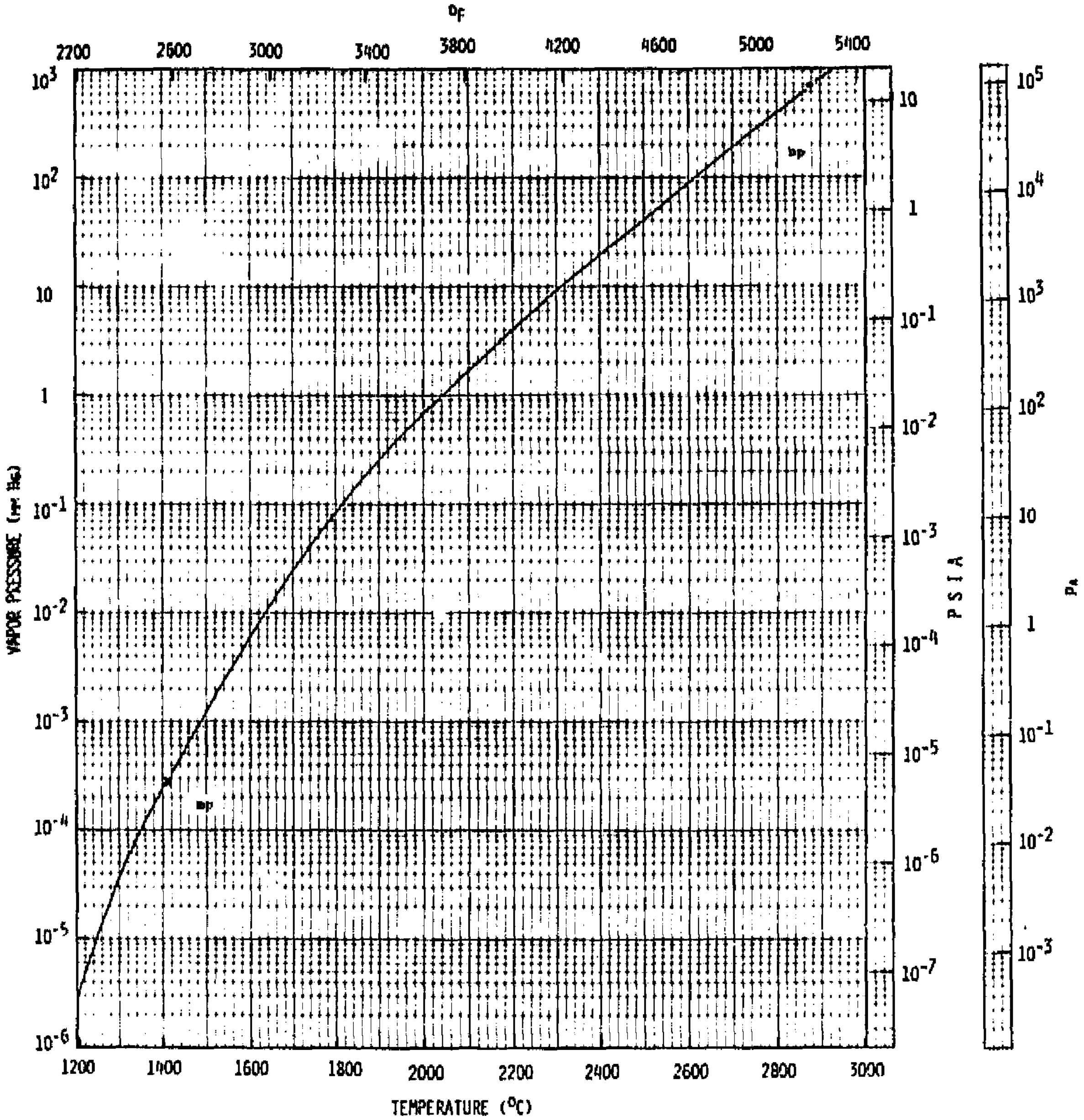

Figure 2.6-1 Vapor Pressure vs Temperature for Silicon

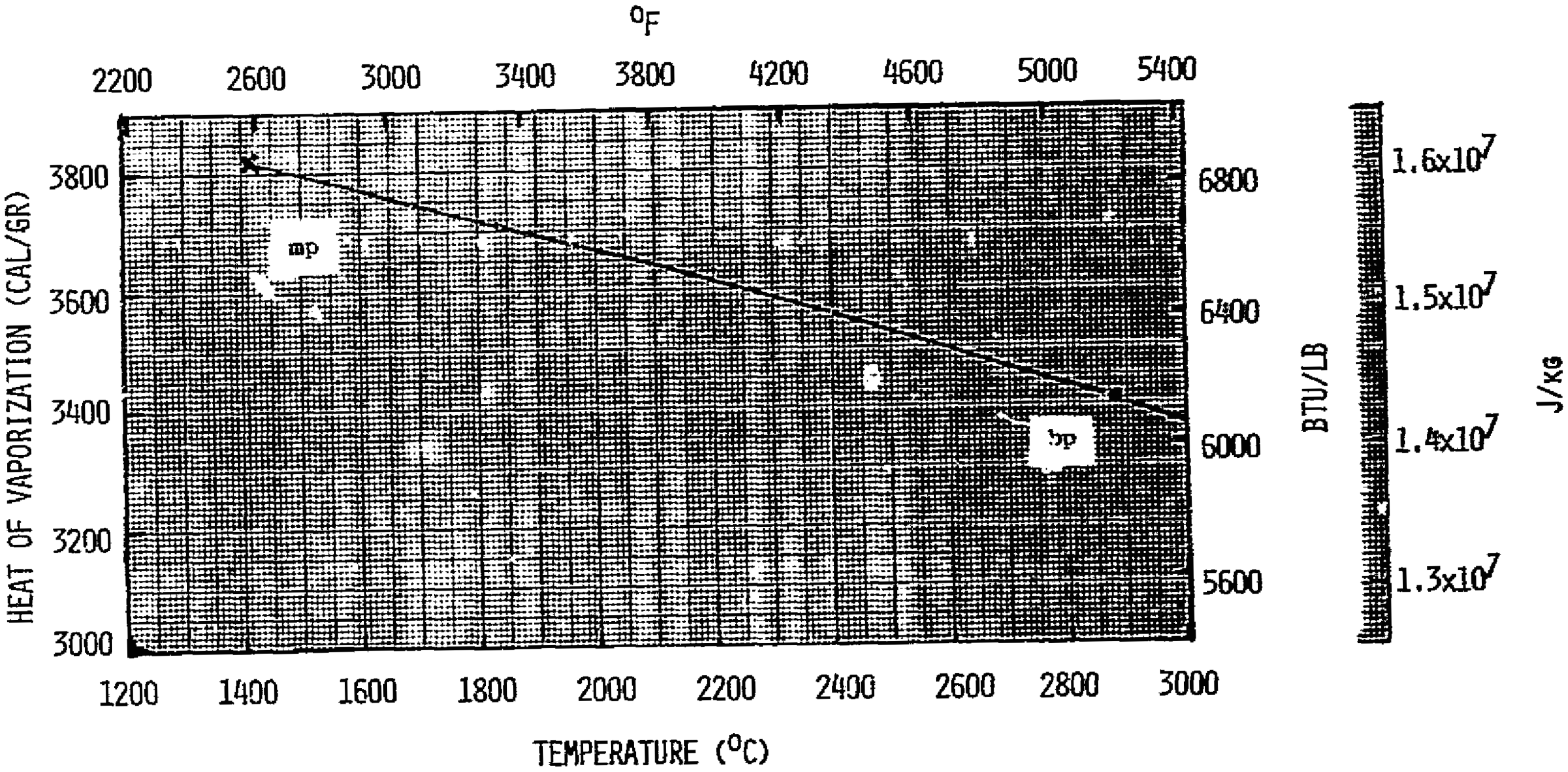

Figure 2.6-2 Heat of Vaporization vs Temperature for Silicon

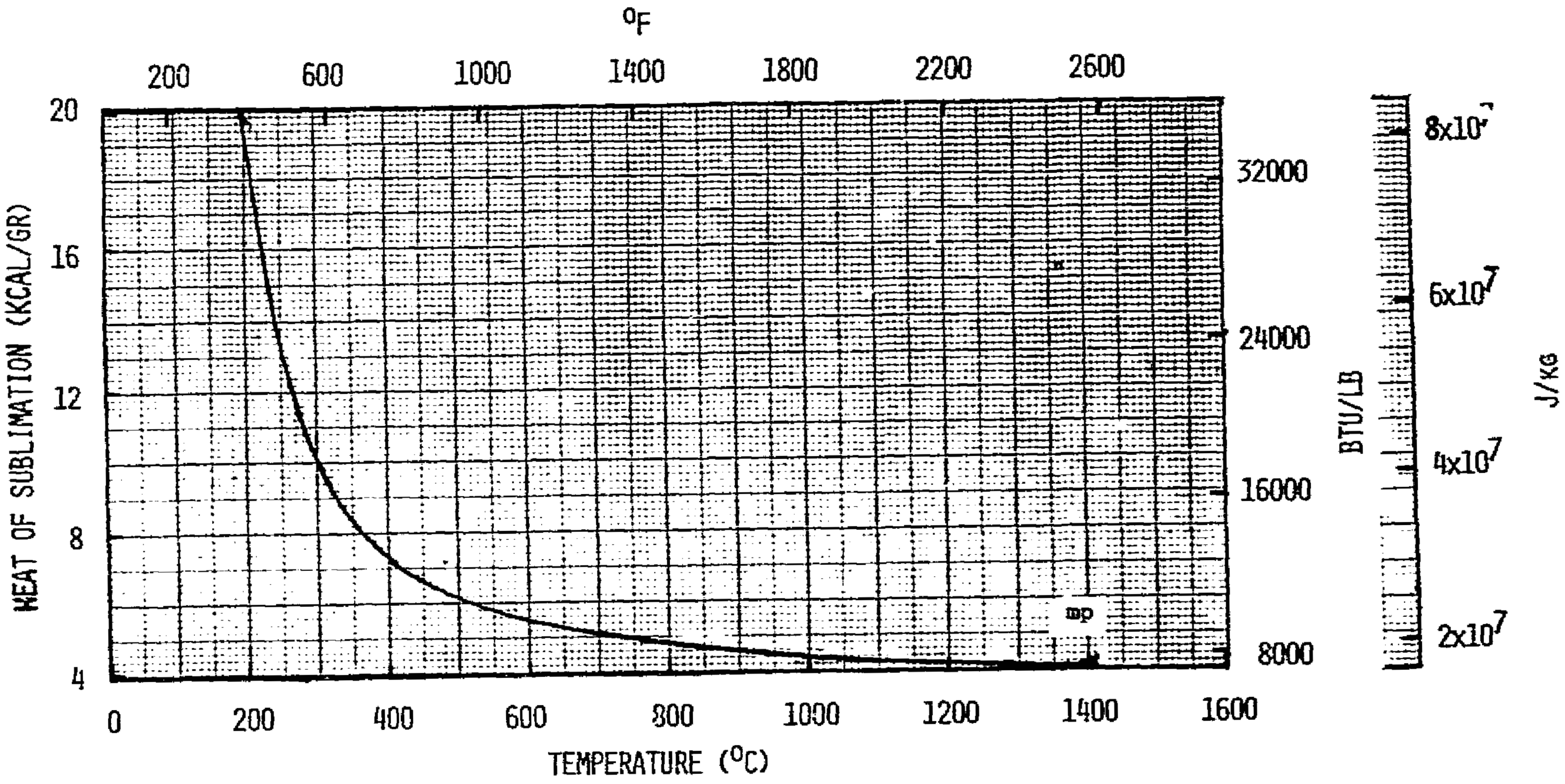

Figure 2.6-3 Heat of Sublimation vs Temperature for Silicon

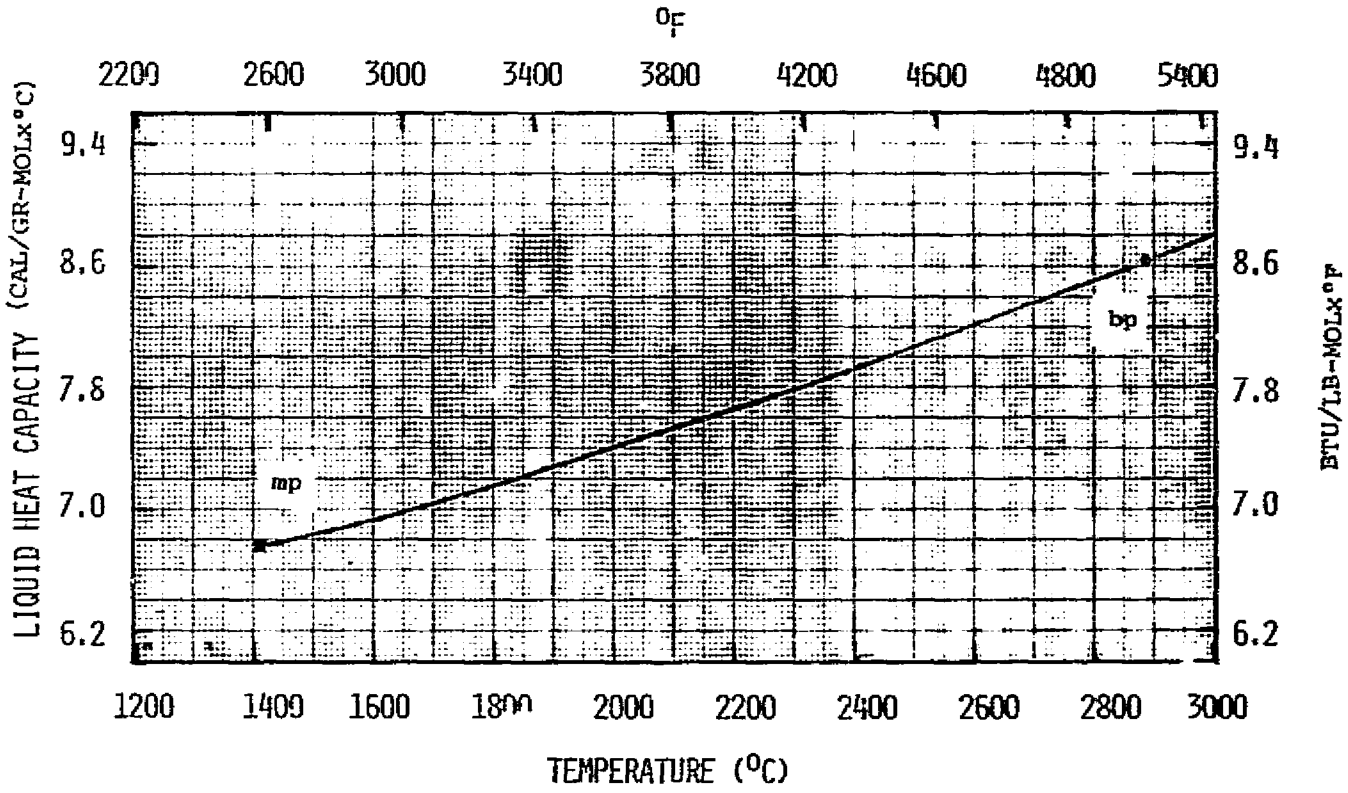

Figure 2.6-4 Liquid Heat Capacity vs Temperature for Silicon

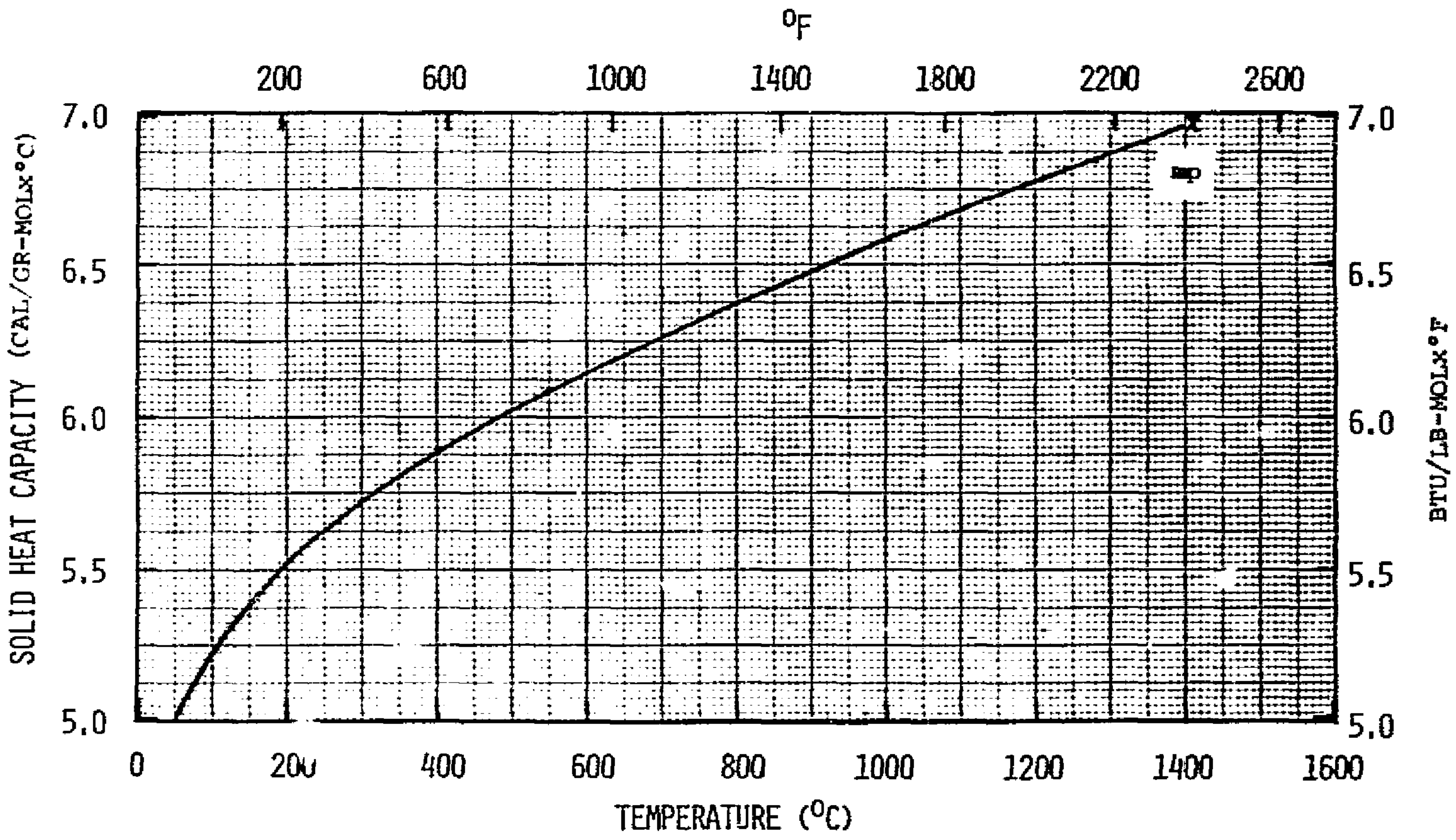

Figure 2.6-5 Solid Heat Capacity vs Temperature for Silicon

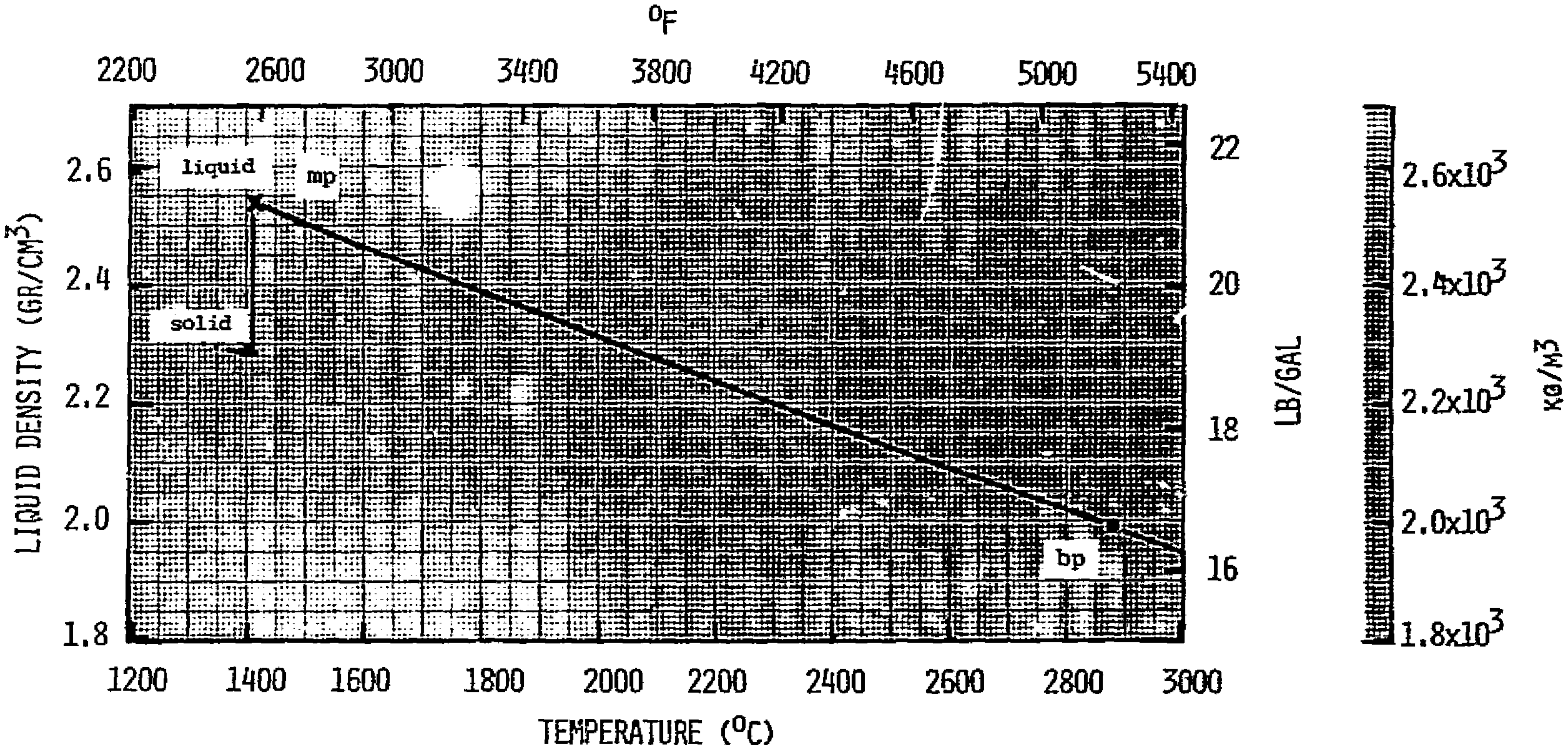

Figure 2.6-6 Liquid Density vs Temperature for Silicon

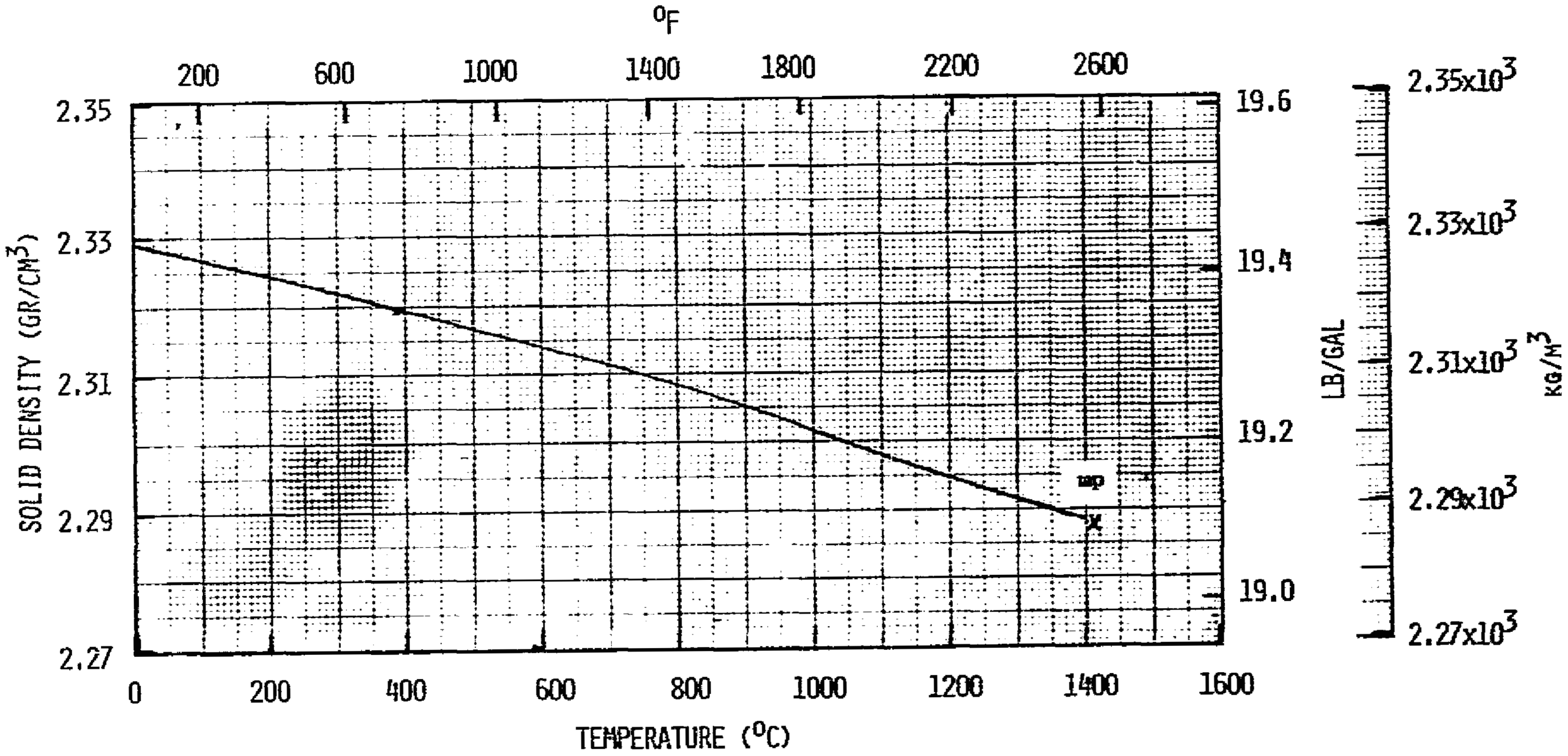

Figure 2.6-7 Solid Density vs Temperature for Silicon

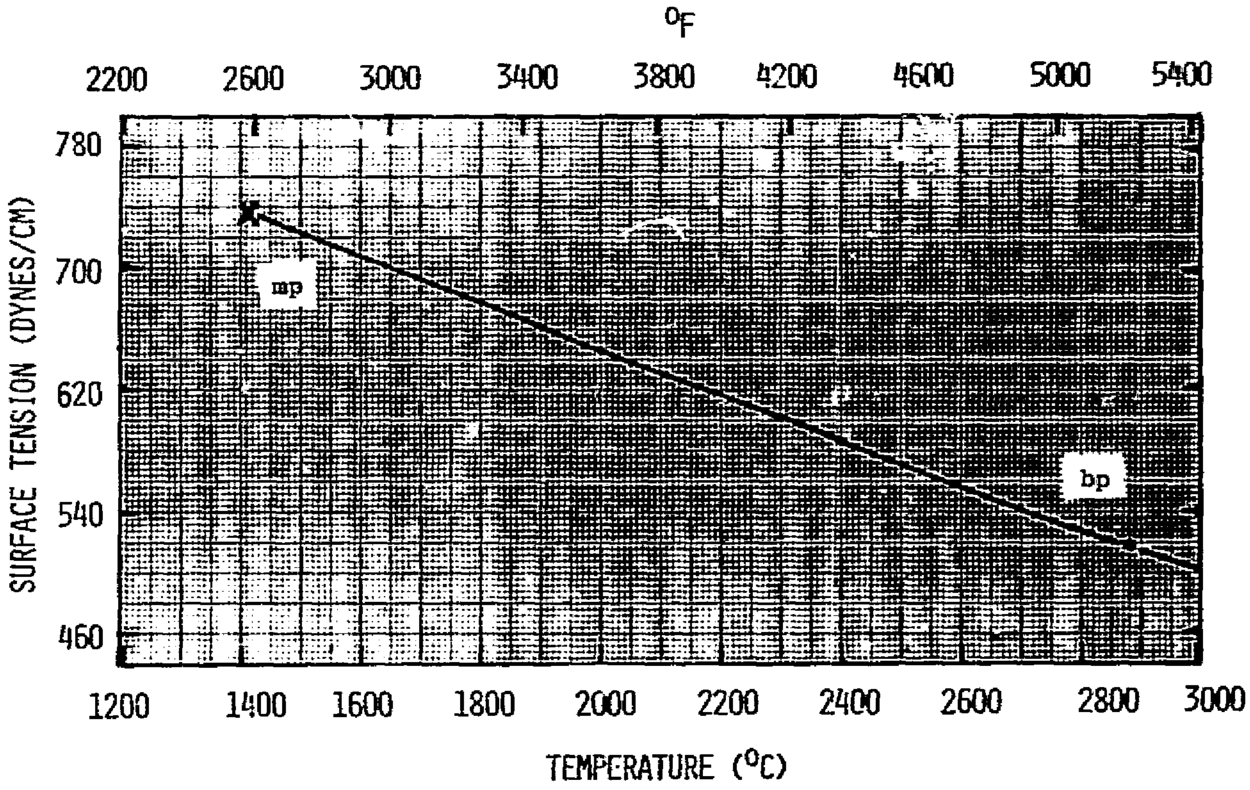

Figure 2.6-8 Surface Tension vs Temperature for Silicon

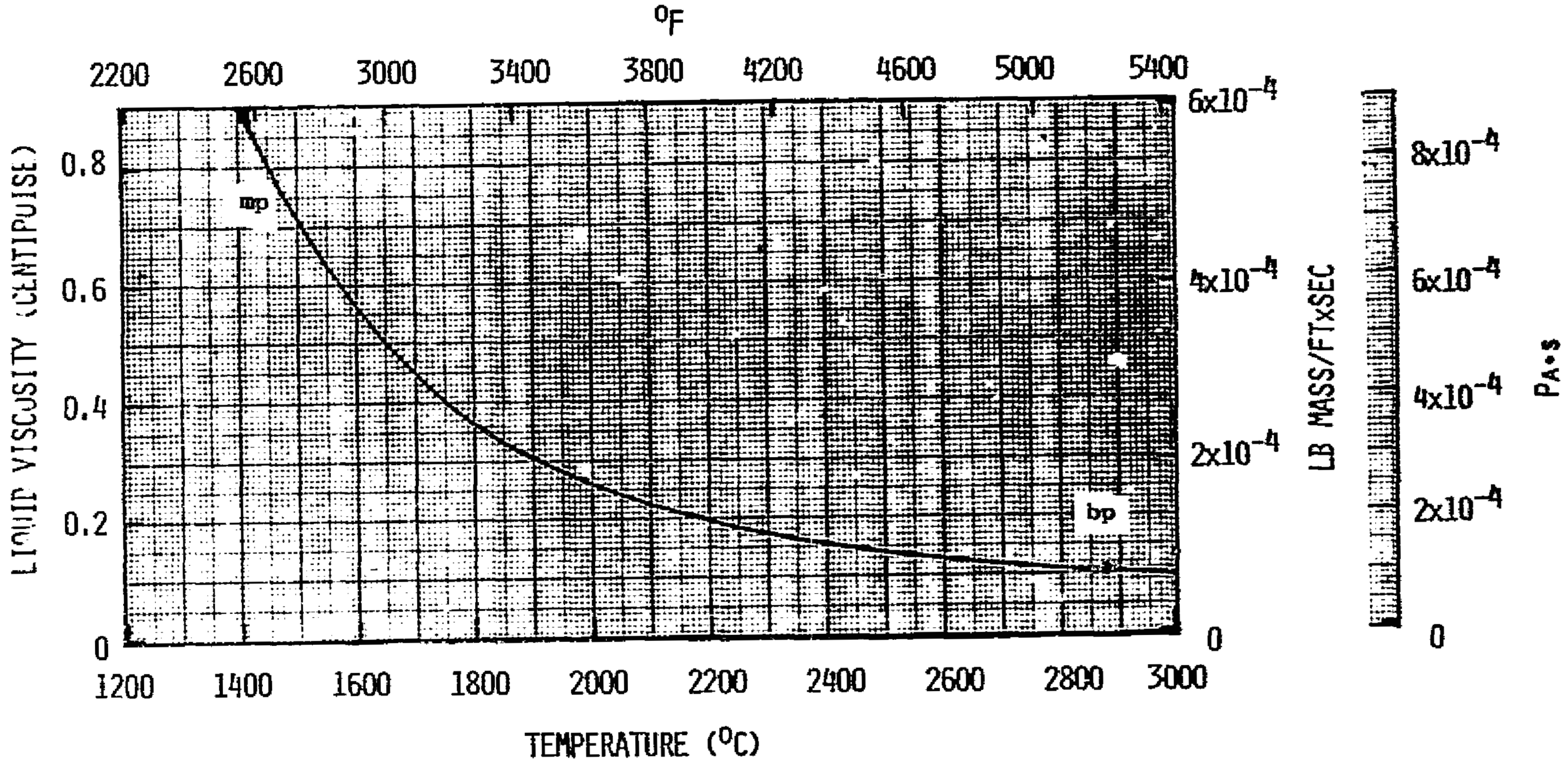

Figure 2.6-9 Liquid Viscosity vs Temperature for Silicon

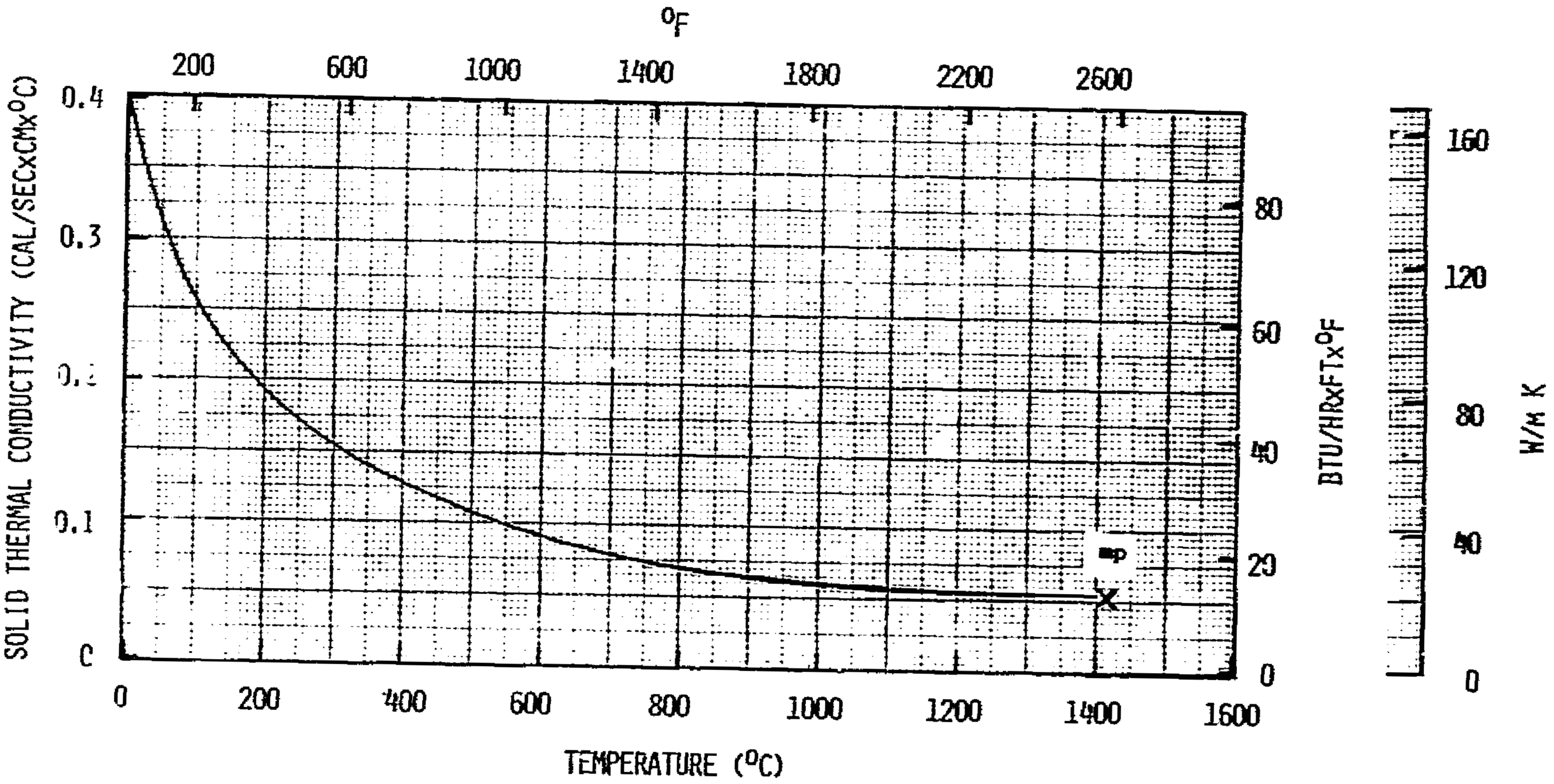

Figure 2.6-10 Solid Thermal Conductivity vs Temperature for Silicon

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2.7 Thermal Conductivity Investigation

Gas phase thermal conductivity values were experimentally determined between 25°C and 350°C for a variety of silicon source materials which included silane and halogenated solanes. The apparatus used was 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 2.7-1). 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.

The thermocouples (type K) used to monitor the temperature of the thermal conductivity cell were calibrated using materials of known melting points throughout the temperature range of the study (25°C to 350°C). The EMF of the thermocouples was measured with a Leeds and Northrup, Model 8686, millivolt potentiometer which was calibrated and certified at the factory. The temperatures reported for the thermal conductivity values are considered to be accurate to ±1°C.

Since absolute measurement of thermal conductivity is difficult, a differential method was employed in which the catharometer was 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 2.7-1: (reference 1)

$$E - E_{ref.} = b({}^{1}/\lambda - {}^{1}/\lambda_{ref}) \qquad (2.7\text{-}1)$$

where E_{ref} is voltage with the reference gas in both sides of the thermal conductivity cell, λ and λ_{ref} are the thermal conductivities of the unknown and reference gas respectively, and b is a constant characteristic of the paricular 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.

Before thermal conductivity data could be obtained, the apparatus described above needed to be calibrated. The calibration work included the determination of cell constants for the temperature range 25°C to 350°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 and hydrogen in the temperature range 25°C to 350°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 were routinely determined everytime data were 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 2.7-2). When thermal conductivity data were being obtained, the filament resistance was routinely calculated by monitoring the current through the filament and the potential across the filament. The filament temperature can then be obtained from figure 2.7-1. The filament current was then adjusted so that the temperature difference between the filament and the cell wall was small.

The thermal conductivity of argon was determined through out the temperature range 25°C to 350°C. These values were compared to recommended values for the thermal conductivity of argon (reference 2) in order to evaluate the accuracy of data obtained on this apparatus (figure 2.7-3). 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 ± 5%. The thermal conductivity values obtained in this study agree with the recommended values to within ± 2% up to 300°C and ± 4% from 300°C to 350°C.

The thermal conductivity of hydrogen was determined in the temperature range 25°C to 350°C. These values were compared to previously reported experimental values for thermal conductivity of hydrogen (references 3 and 4) in order to evaluate the accuracy of the data obtained on this apparatus (figure 2.7-4) for gases of relatively high thermal conductivity.

The thermal conductivity of silane (SiH_4) was determined between 25°C and 300°C (Table 2.7-1 and Figure 2.7-5). Values above 300°C were not determined because above that temperature silane is thermally unstable and begins to deposit silicon. There have been no previously reported experimental data for gaseous thermal conductivity of silane. Estimated values have been determined using a modified Eucken Correlation (ref. 5) and these estimated values agree fairly well with the now available experimental values.

The thermal conductivity of dichlorosilane (SiH_2Cl_2) was determined between 25°C and 350°C (Table 2.7-2 and Figure 2.7-6). There have been no previously reported experimental data for gaseous thermal conductivity of dichlorosilane. Estimated values have been reported (reference 39) in the temperature range 0°C to 70°C which were determined by a Euchen approximation. These estimated values are considerably lower than the experimental values now reported.

The thermal conductivity of trichlorosilane ($SiHCl_3$) was determined between 50°C and 350°C (Table 2.7-3 and Figure 2.7-7). There have been no previously reported experimental data for gaseous thermal conductivity of trichlorosilane.

The thermal conductivity of gaseous silicon tetrachloride was determined between 100°C and 350°C (Table 2.7-4 and Figure 2.7-8). There have been both calculated (ref. 7) and experimental (ref. 8) values for the thermal conductivity of silicon tetrachloride previously reported. The calculated values, in the temperature range 80°C to 335°C, were lower than the values obtained in this study by more than 10%. The experimental values, in the temperature range 70°C to 300°C, were about 10% lower than the values obtained in this study.

The thermal conductivity of silicon tetrafluoride (SiF_4) was determined beween 25° and 350°C (Table 2.7-5 and Figure 2.7-9). The values obtained in this study agree to wtihin ±3% with previously reported (reference 9) experimental data for silicon tetrafluoride (figure 2.7-10)

Figure 2.7-11 summarizes all of the experimentally determined values for gaseous thermal conductivity of silane and halogenated silanes reported from this investigation.

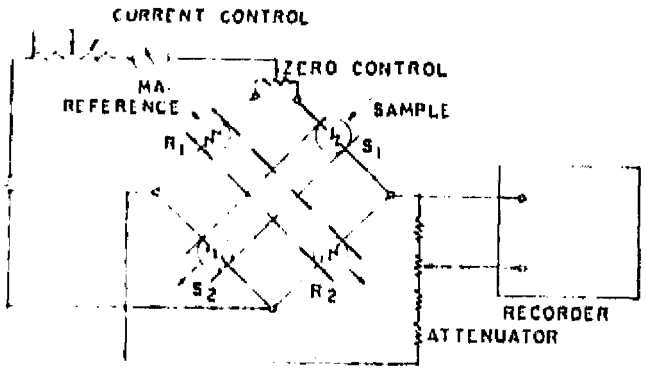

Figure 2.7-1 Wheatstone Bridge Circuit For Thermal Conductivity Cell

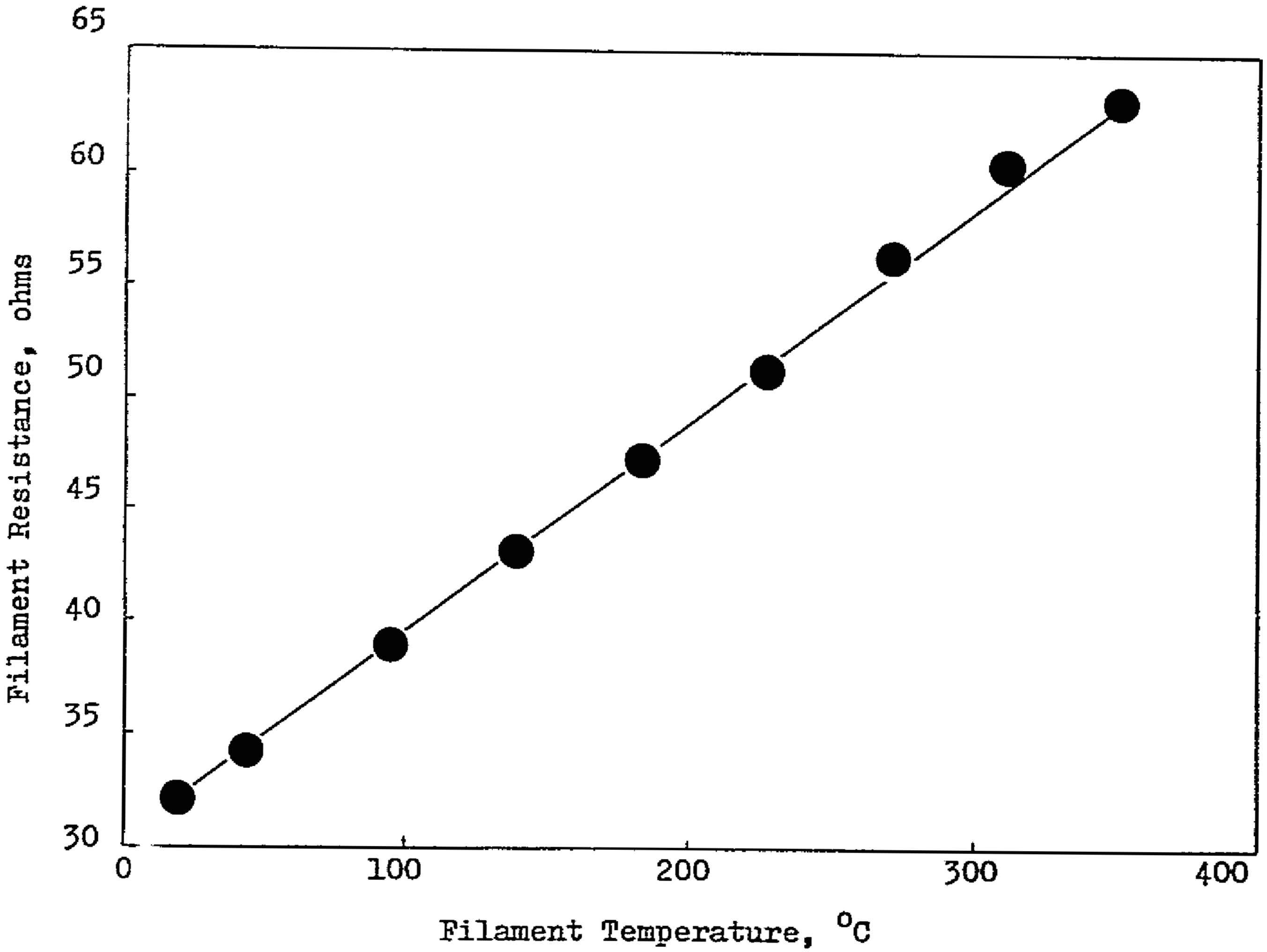

Figure 2.7-2 Filament Resistance as a Function of Temperature

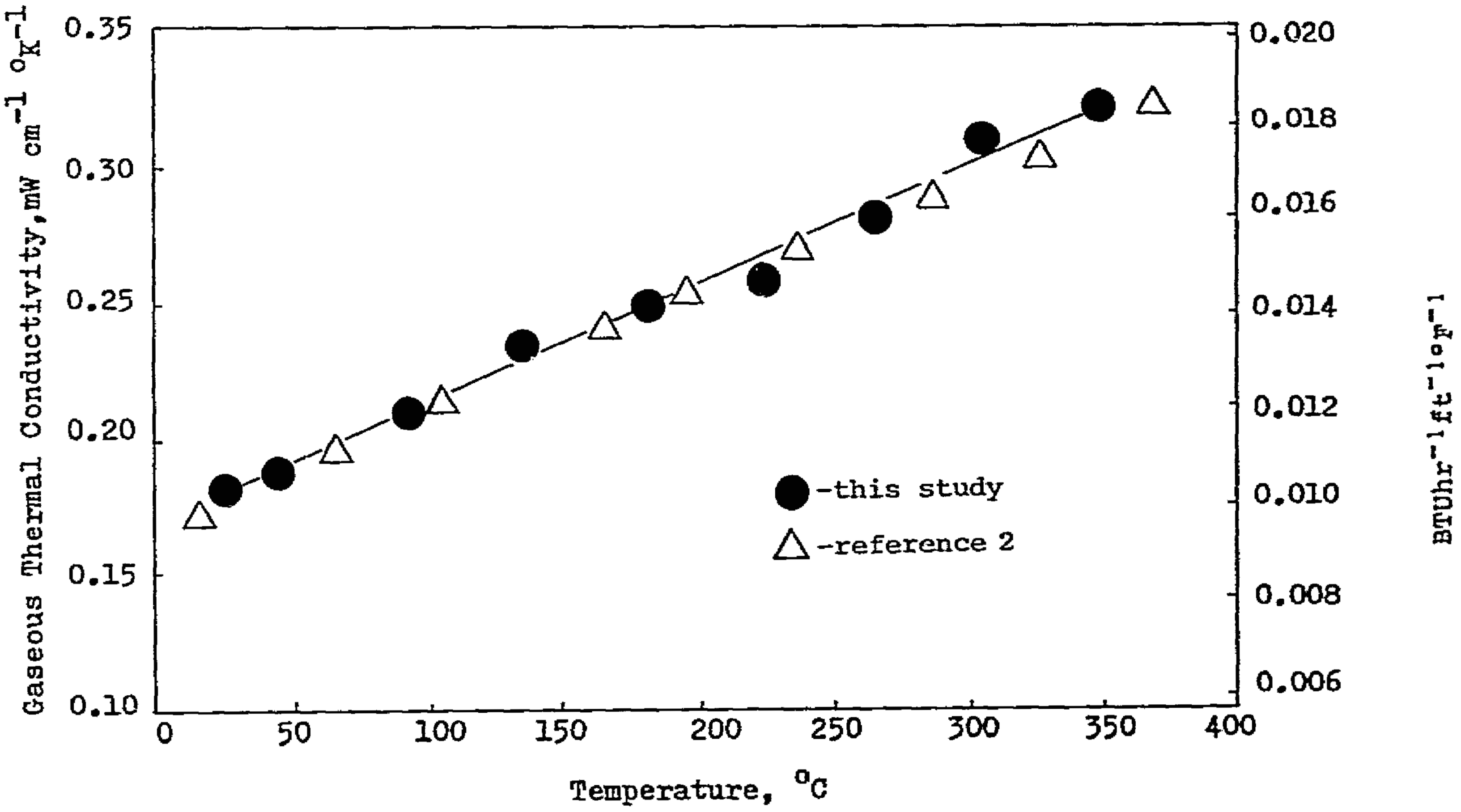

Figure 2.7-3 Comparison of Thermal Conductivity Values for Argon

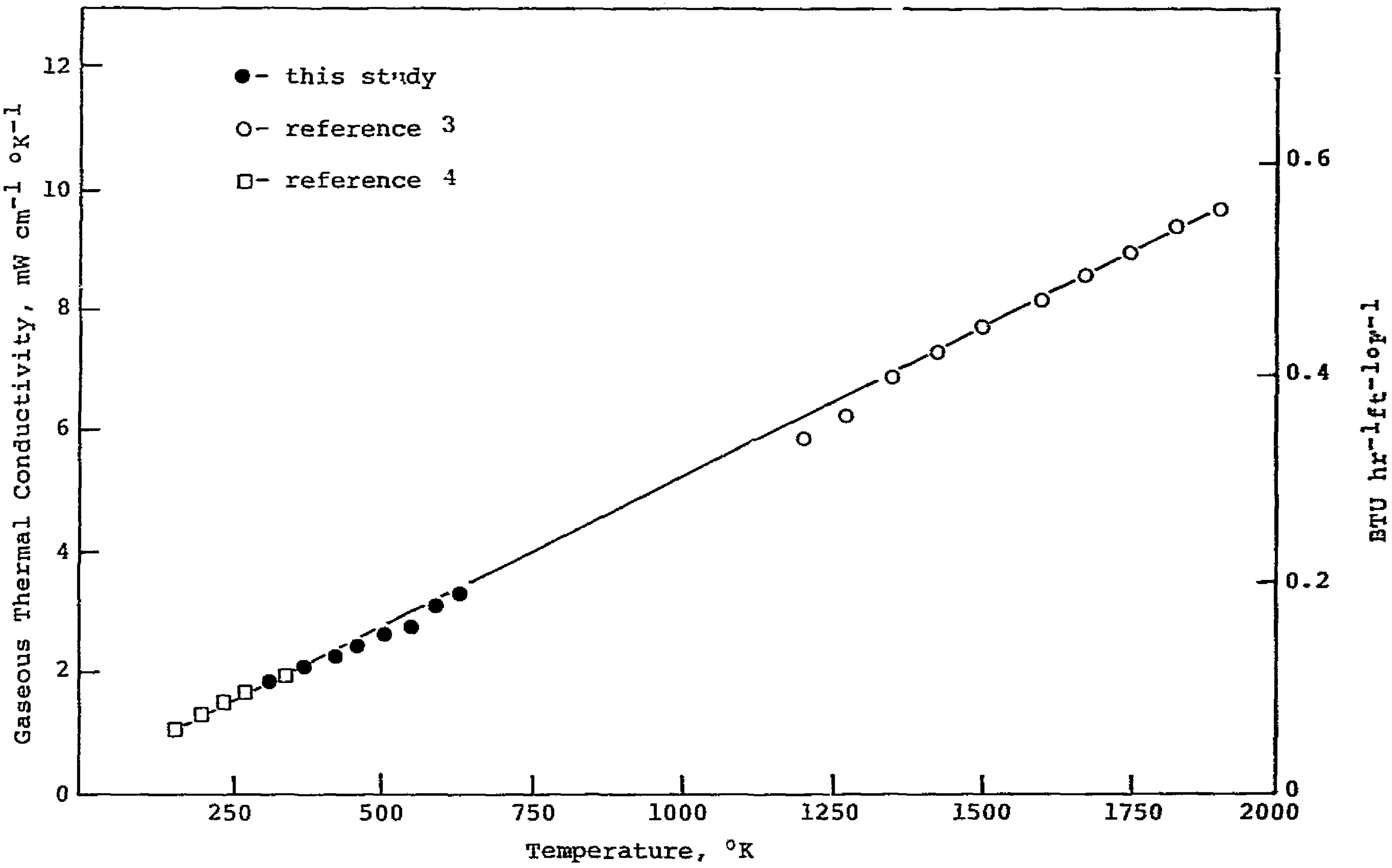

Figure 2.7-4 Comparison of Thermal Conductivity Values for Hydrogen

Table 2.7-1 Gaseous Thermal Conductivity Values of Silane

Temperature	Gaseous Thermal Conductivity		
^{o}C	$mW\ cm^{-1}\ {}^{o}K^{-1}$	$Cal\ cm^{-1} sec^{-1}\ {}^{o}C^{-1}$	$BTU\ hr^{-1} ft^{-1}\ {}^{o}F^{-1}$
28.0	0.234	56.02×10^{-6}	13.54×10^{-3}
45.7	0.249	59.44×10^{-6}	14.37×10^{-3}
94.7	0.297	70.96×10^{-6}	17.15×10^{-3}
139.4	0.345	82.34×10^{-6}	19.90×10^{-3}
184.1	0.400	95.67×10^{-6}	23.13×10^{-3}
227.4	0.449	107.24×10^{-6}	25.93×10^{-3}
269.5	0.497	118.86×10^{-6}	28.73×10^{-3}

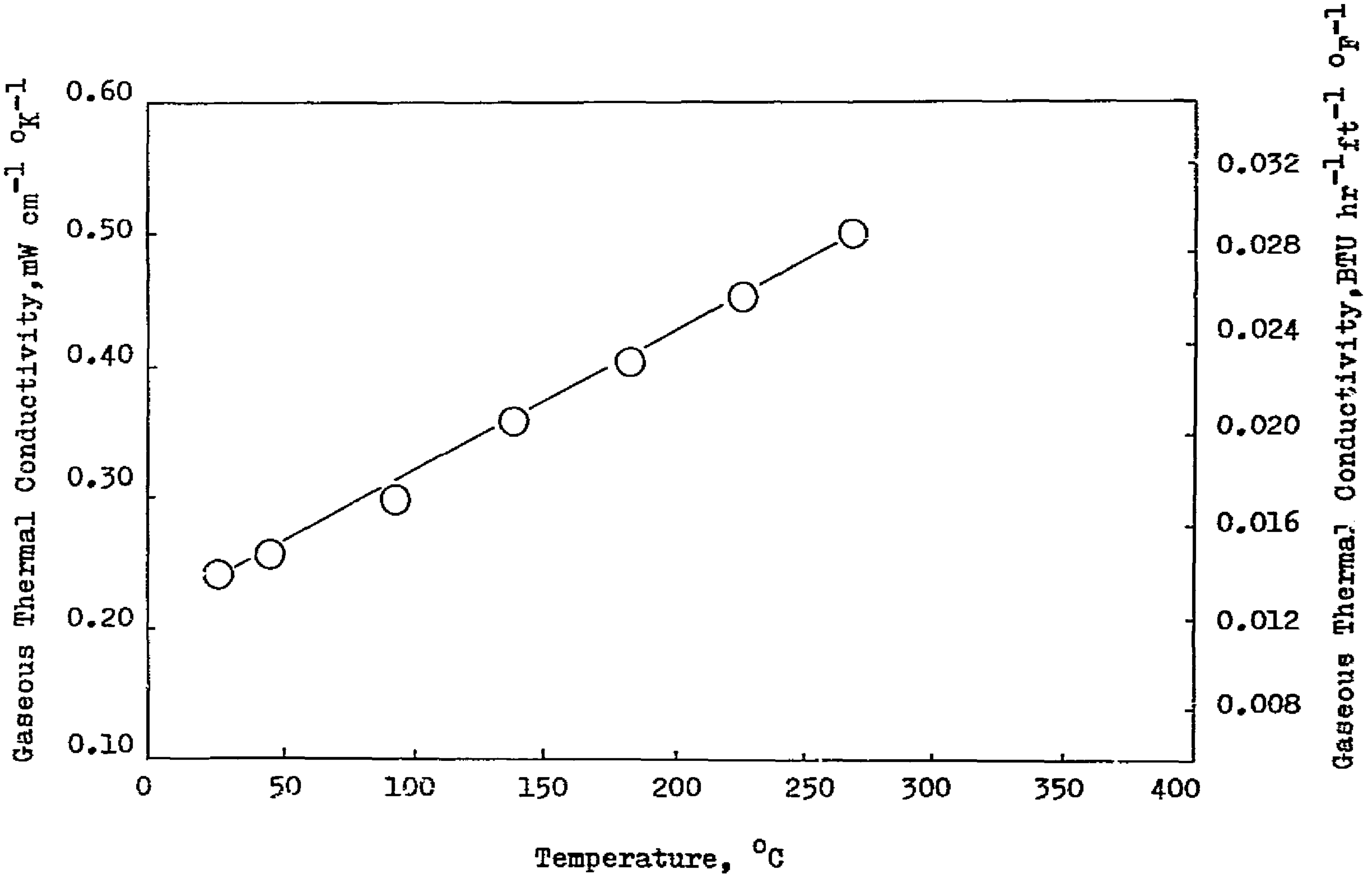

Figure 2.7-5 Gaseous Thermal Conductivity of Silane

Table 2.7-2 Gaseous Thermal Conductivity Values of Dichlorosilane

Temperature	Gaseous Thermal Conductivity		
°C	mW cm^{-1} °K^{-1}	Cal cm^{-1}sec^{-1} °C^{-1}	BTU hr^{-1}ft^{-1} °F^{-1}
28.0	0.102	24.43 X 10^{-6}	5.91 X 10^{-3}
45.7	0.108	25.72 X 10^{-6}	6.22 X 10^{-3}
94.7	0.129	30.86 X 10^{-6}	7.46 X 10^{-3}
139.4	0.148	35.42 X 10^{-6}	8.56 X 10^{-3}
184.1	0.169	40.37 X 10^{-6}	9.76 X 10^{-3}
[illegible]7.4	0.194	46.46 X 10^{-6}	11.23 X 10^{-3}
[illegible].5	0.217	51.79 X 10^{-6}	12.52 X 10^{-3}
[illegible]1.3	0.243	58.15 X 10^{-6}	14.06 X 10^{-3}
[illegible]30.6	0.267	63.70 X 10^{-6}	15.40 X 10^{-3}

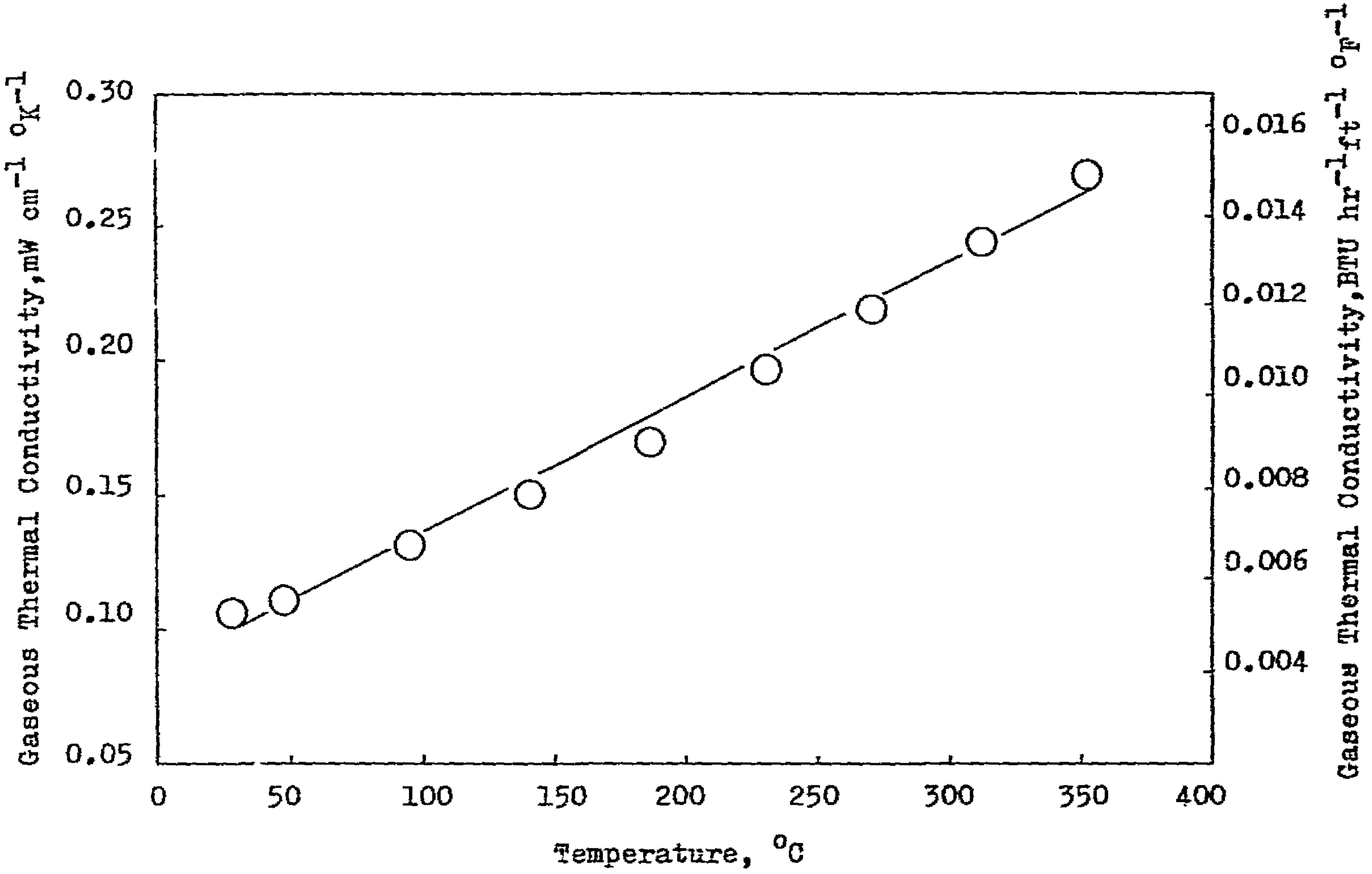

Figure 2.7-6 Gaseous Thermal Conductivity of Dichlorosilane

Table 2.7-3 Gaseous Thermal Conductivity Values of Trichlorosilane

Temperature	Gaseous Thermal Conductivity		
^{o}C	$mW\ cm^{-1}\ {}^{o}K^{-1}$	$Cal\ cm^{-1} sec^{-1}\ {}^{o}C^{-1}$	$BTU\ hr^{-1} ft^{-1}\ {}^{o}F^{-1}$
45.7	0.093	22.13×10^{-6}	5.35×10^{-3}
94.7	0.110	26.22×10^{-6}	6.34×10^{-3}
139.4	0.126	30.16×10^{-6}	7.29×10^{-3}
184.1	0.144	34.35×10^{-6}	8.30×10^{-3}
227.4	0.161	38.55×10^{-6}	9.32×10^{-3}
269.5	0.180	43.05×10^{-6}	10.41×10^{-3}
311.3	0.198	47.24×10^{-6}	11.42×10^{-3}
350.6	0.216	51.58×10^{-6}	12.47×10^{-3}

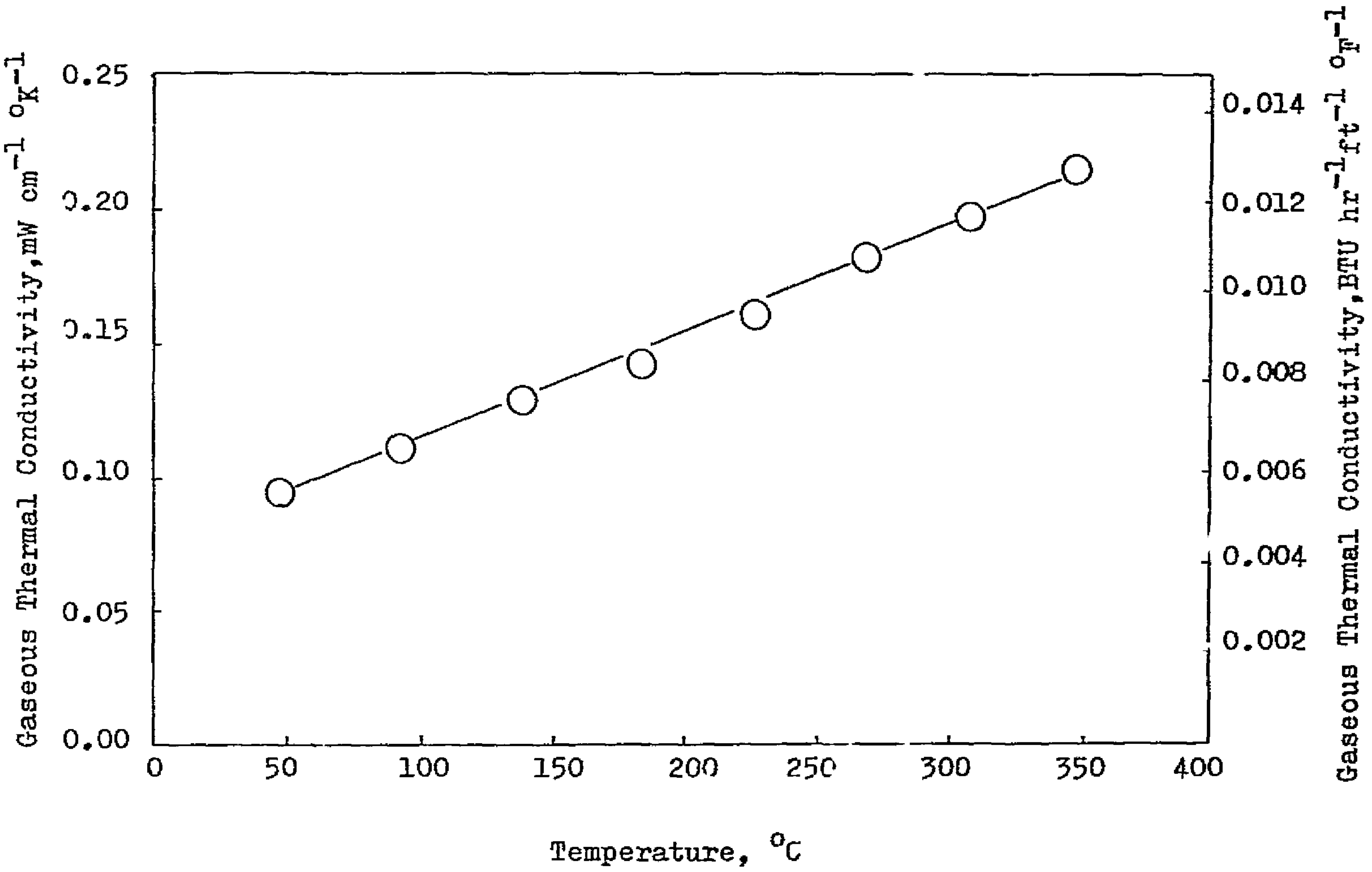

Figure 2.7-7 Gaseous Thermal Conductivity of Trichlorosilane

Table 2.7-4 Gaseous Thermal Conductivity Values of Tetrachlorosilane

Temperature	Gaseous Thermal Conductivity		
^{o}C	mW cm^{-1} ^{o}K^{-1}	Cal cm^{-1}sec^{-1} ^{o}C^{-1}	BTU hr^{-1}ft^{-1} ^{o}F^{-1}
94.7	0.100	23.93 X 10^{-6}	5.78 X 10^{-3}
139.4	0.111	26.43 X 10^{-6}	6.39 X 10^{-3}
184.1	0.124	29.59 X 10^{-6}	7.15 X 10^{-3}
227.4	0.138	32.89 X 10^{-6}	7.95 X 10^{-3}
269.5	0.153	36.59 X 10^{-6}	8.85 X 10^{-3}
311.3	0.169	40.39 X 10^{-6}	9.76 X 10^{-3}
350.6	0.193	46.13 X 10^{-6}	11.15 X 10^{-3}

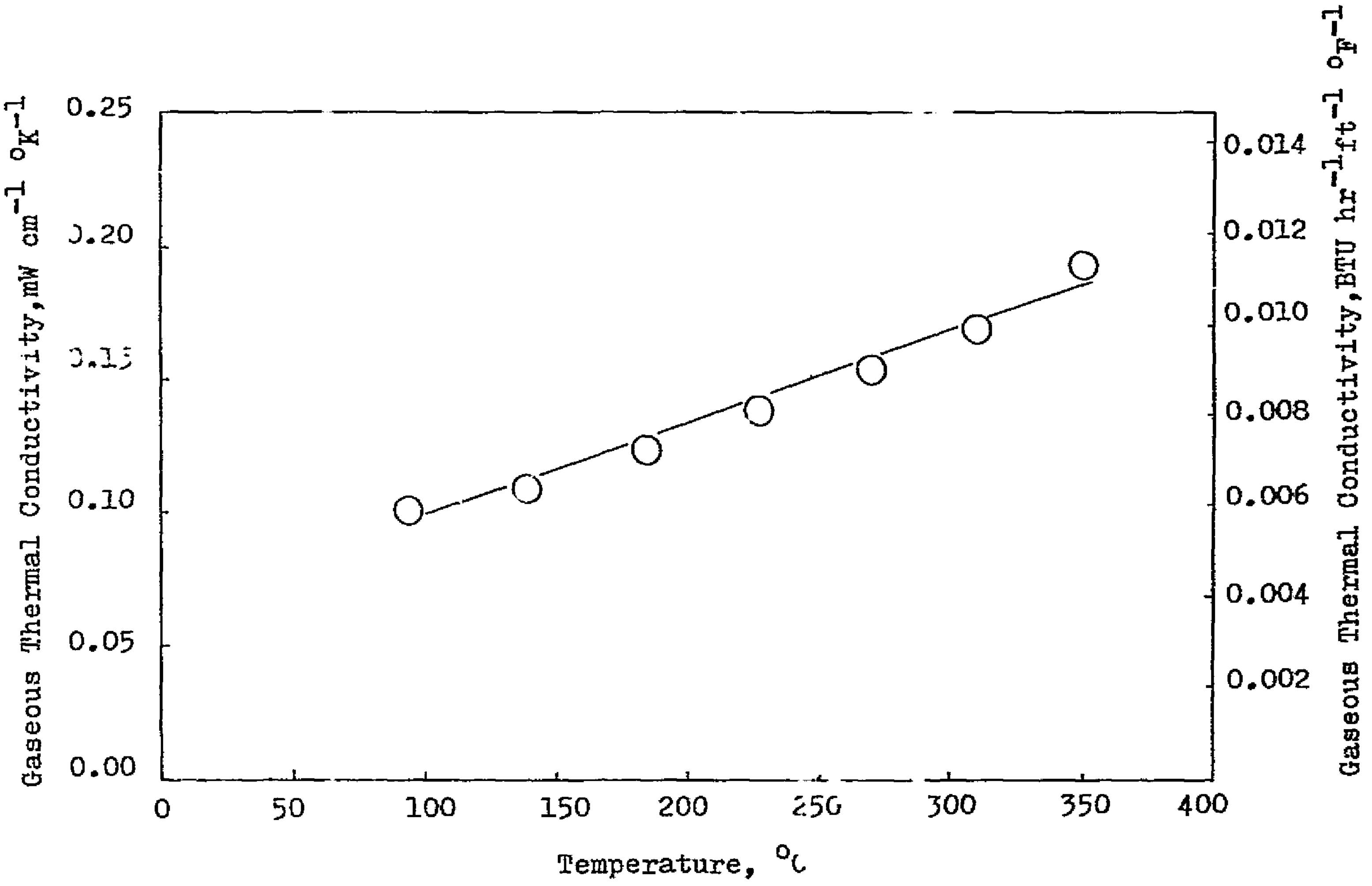

Figure 2.7-8 Gaseous Thermal Conductivity of Tetrachlorosilane

Table 2.7-5 Gaseous Thermal Conductivity Values of Tetrafluorosilane

Temperature	Gaseous Thermal Conductivity		
°C	mW cm^{-1} °K^{-1}	Cal cm^{-1}sec^{-1} °C^{-1}	BTU hr^{-1}ft^{-1} °F^{-1}
29.0	0.150	35.95 X 10^{-6}	8.69 X 10^{-3}
45.7	0.158	37.79 X 10^{-6}	9.13 X 10^{-3}
94.7	0.189	45.24 X 10^{-6}	10.94 X 10^{-3}
139.4	0.215	51.43 X 10^{-6}	12.43 X 10^{-3}
184.1	0.241	57.67 X 10^{-6}	13.94 X 10^{-3}
227.4	0.274	65.46 X 10^{-6}	15.83 X 10^{-3}
269.5	0.291	69.55 X 10^{-6}	16.81 X 10^{-3}
311.3	0.316	75.55 X 10^{-6}	18.26 X 10^{-3}
350.6	0.345	82.34 X 10^{-6}	19.90 X 10^{-3}

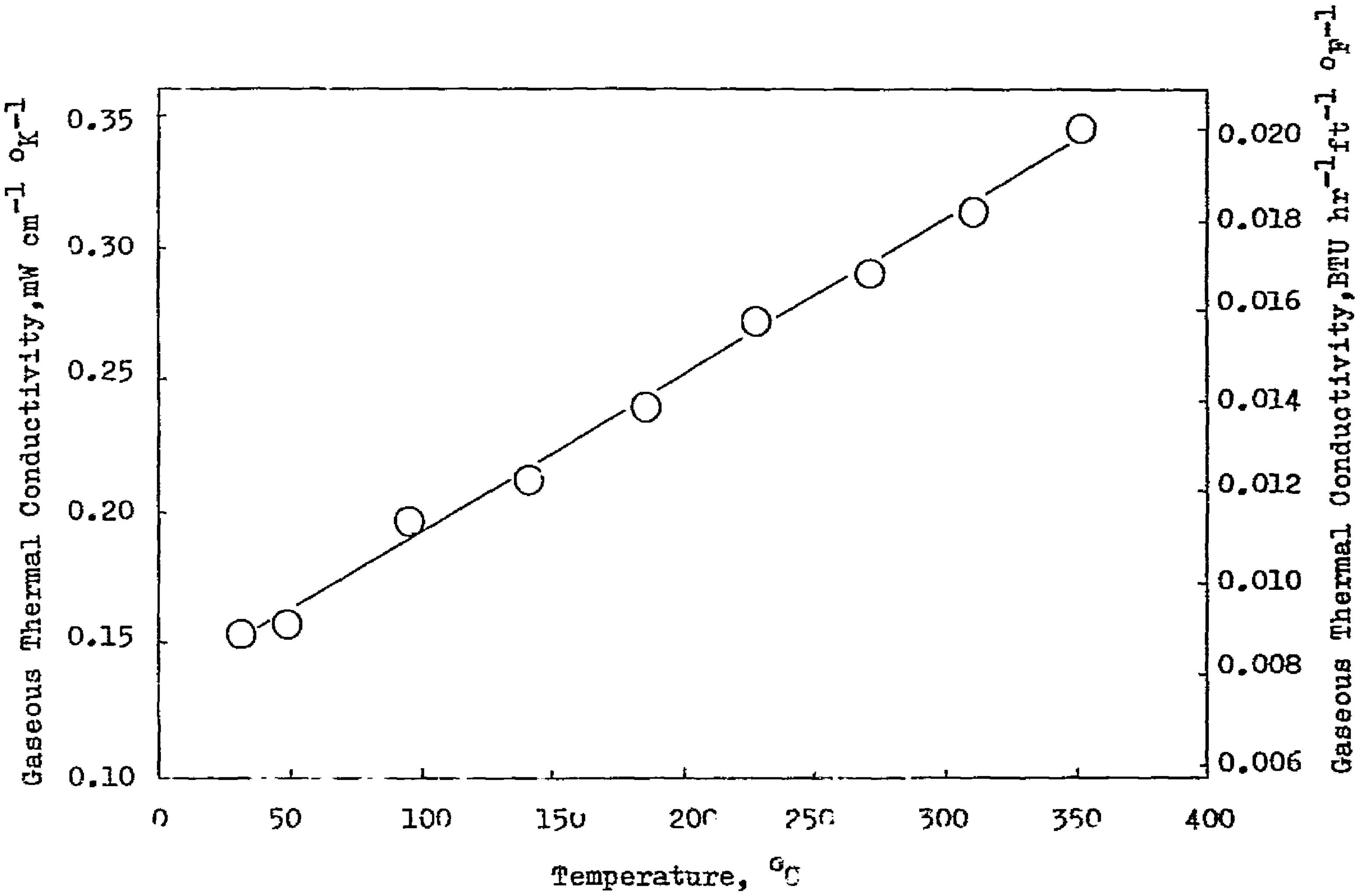

Figure 2.7-9 Gaseous Thermal Conductivity of Tetrafluorosilane

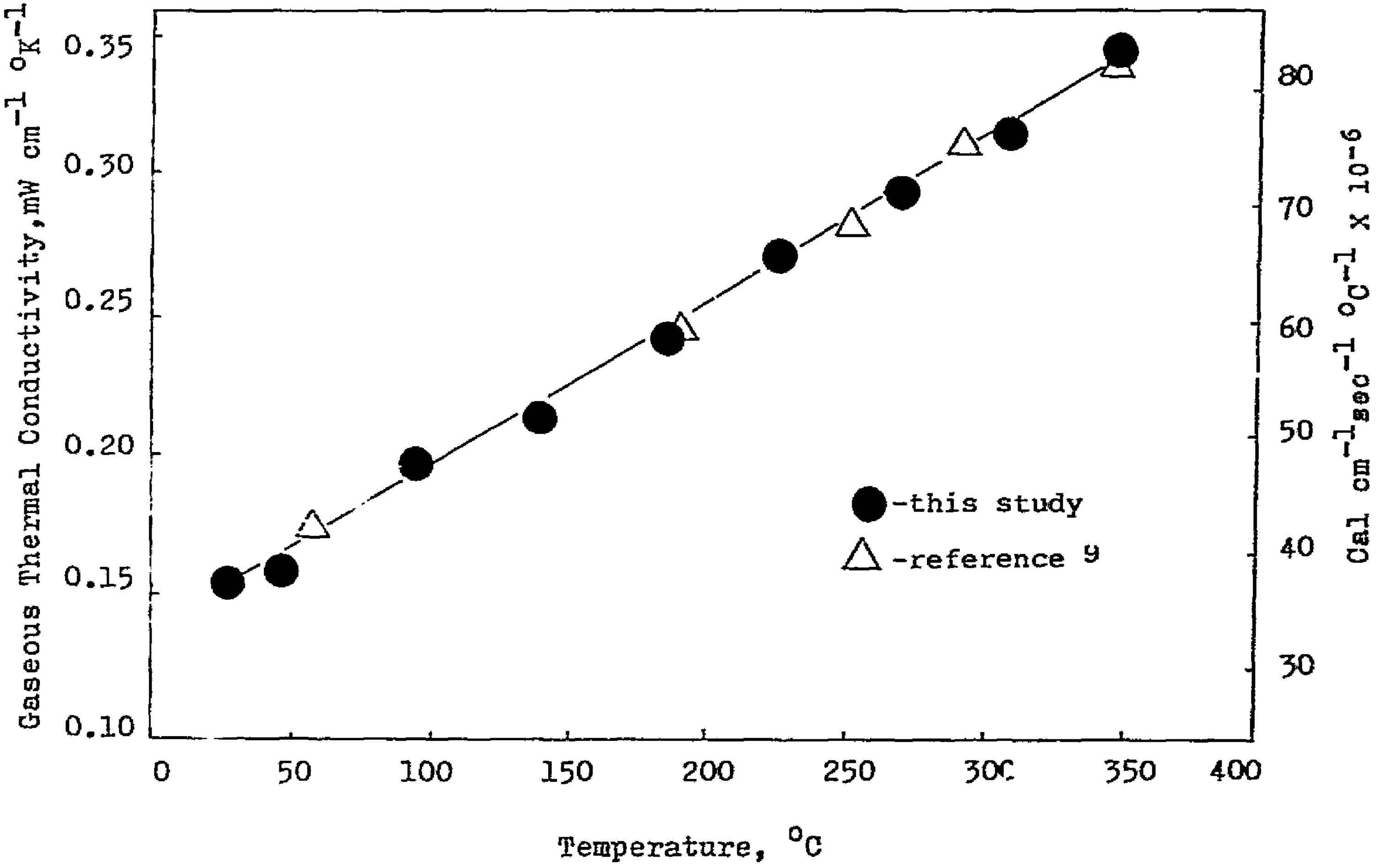

Figure 2.7-10 Comparison of Thermal Conductivity Values for Tetrafluorosilane

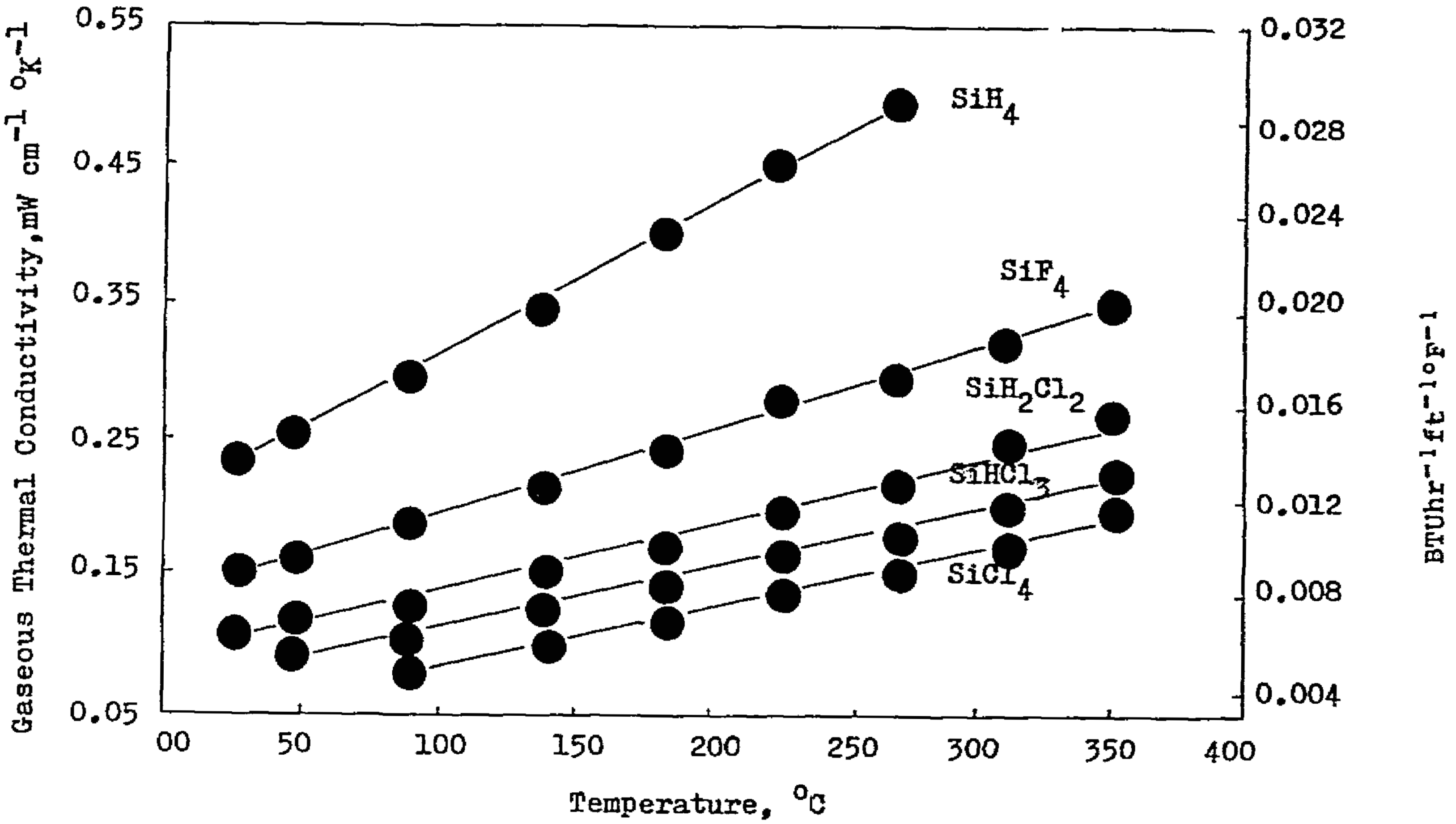

Figure 2.7-11 Gaseous Thermal Conductivity Values for Silane and Halogenated Silanes

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2.8 Viscosity Investigation

Gas viscosity values of some halogenated silanes were experimentally determined between 40°C and 200°C. The viscosity values were determined by a transpiration method which is based on the rate of flow of the gas through a capillary. In order to determine these gas flow rates, a constant volume, glass viscometer (Figure 2.8-1) was fabricated and assembled. The apparatus is similar to one described by McCoubrey and Singh (1). The apparatus consist of a 1 liter glass bulb which is connected through a glass manifold to a mercury manometer and to a thermostated capillary with a preheater coil. The capillary is 20 cm. in length and has an internal diameter of 0.02 cm. The exit side of the capillary can be continuously evacuated by a two stage mechanical pump.

In order to make a measurement, the viscometer is thoroughly evacuated and then the gas sample is introduced into the bulb up to a pressure of about 18 cm. Hg. The gas sample is then evacuated through the capillary and the resulting rate of flow is monitored by recording the pressure decrease in the bulb with time. The pressure is measured with a standard U tube mercury manometer to ±0.5mm. Hg.

The rate of flow of a gas through a capillary is dependent upon the coefficient of viscosity (η) of the gas. By combining Poiseuille's equation for laminar flow of a gas through a tube and the ideal gas law equation: the relationship between pressure, time, and viscosity of a gas can be derived. Poiseuille's equation (2) for laminar gas flow is:

$$\frac{dV}{dt} = \frac{\pi(P_1^2 - P_2^2)r^4}{16L\eta P_0} \qquad (2.8\text{-}1)$$

where dV/dt is the volume rate of gas flowing through the capillary, P_1 is the pressure at the capillary inlet, P_2 is the pressure at the capillary outlet, r is the radius of the capillary, L is the length of the capillary, and P_0 is the pressure at which the gas volume is measured. In this method where the gas is continuously evacuated with a pump, P_2 is negligible compared to P_1 and equation 2.8-1 reduces to:

$$\frac{dV}{dt} = \frac{\pi P_1^2 r^4}{16L\eta P_0} \qquad (2.8\text{-}2)$$

From the ideal gas law, dV, the volume of gas at P_0, passing through the capillary in unit time can be expressed in terms of dN, the number of moles of gas flowing through the capillary in unit time (equation 2.8-3).

$$dV = dN(RT/P_0) \qquad (2.8\text{-}3)$$

Substituting equation 2.8-3 into equation 2.8-2 gives equation 2.8-4:

$$\frac{dN}{dt} = \frac{\pi P_1^2 r^4}{16 L \eta R T} \qquad (2.8\text{-}4)$$

As the gas is evacuated in a constant volume viscometer, the pressure decreases. Again using the ideal gas law,

$$dN = -dP_1(V/RT) \qquad (2.8\text{-}5)$$

where V is the volume being evacuated. Substituting equation 2.8-5 into equation 2.8-4 gives equation 2.8-6

$$dP_1 = \frac{-\pi P_1^2 r^4}{16 L \eta V}\, dt \qquad (2.8\text{-}6)$$

The assumptions of the derivations are: constant volume of the system, ideal behavior of the gas, and laminar flow through the capillary. Since the pressure is measured with a U-tube manometer the volume of the system will change by 10 to 20 ml. during an experiment. However, with a total volume of the viscometer of over 1 liter, this change can be neglected. The gases to be measured do not exhibit ideal behavior, but at pressures of less than 1 atmosphere their deviations should not be large. Laminar flow assumes zero velocity at the wall. A correction may need to be made for slip at the wall.

From equation 2.8-6, the viscosity (η) of a gas can be calculated from the slope of the line obtained by plotting $1/P_1$ versus t. In order to avoid the necessity of careful measurements of the capillary dimensions and the volume of the system a gas of known viscosity can be used to determine an apparatus constant which includes all the constant terms in equation 2.8-6. Alternatively, the calculation constant can be omitted and the viscosity of the unknown, relative to that of a reference gas, can be computed from the inverse ration of the slopes of the 1/P versus t graphs (equation 2.8-7).

$$\frac{\eta}{\eta_{ref}} = \frac{slope_{ref}}{slope} \qquad (2.8\text{-}7)$$

Evaluation and calibration of the gas viscometer was accomplished before data collection begun. Using argon as a reference to determine a viscometer constant, experimental values for gas viscosity of nitrogen have been determined between 40°C and 200°C. These values were compared to recommended values for the gas viscosity of nitrogen (3) in order to evaluate the accuracy of data obtained on this viscometer (figure 2.8-2). The recommended values used were those presented in "Thermophysical Properties of Matter", Vol. 11 on viscosity (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 ±2%. The viscosity values obtained for gaseous nitrogen in this study deviate from the recommended values by less than 2% from 40°C 200°C (figure 2.8-2).

The viscosity of trichlorosilane ($SiHCl_3$) has been determined between 40°C and 200°C (table 2.8-1 and figure 2.8-3). There have been no previously reported experimental values for gas viscosity of trichlorosilane in the temperature range of the study. Values at 0°C and 31°C were reported by Tel'chuk and Tubyanskaya (ref. 5).

The viscosity of dichlorosilane (SiH_2Cl_2) has been determined between 40°C and 200°C (table 2.8-2 and figure 2.8-4). The sample of dichlorosilane used for the measurements was semiconductor grade obtained from Union Carbide Corporation. There have been no previously reported experimental values for the gas phase viscosity of dichlorosilane. One set of calculated values have been reported (ref. 6) in the temperature range of 0°C to 300°C. These calculated values agree with the experimental values determined in this study with deviations of less than ±2% from 40°C to 200°C.

The viscosity of tetrafluorosilane (SiF_4) has been determined between 40°C and 200°C (Table 2.8-3 and Figure 2.8-5). There have been two previous reports of experimentally determined viscosity values for tetrafluorosilane. Ellis and Raw (reference 4) reported values between 23°C adn 134°C and McCoubrey and Singh (reference 1) reported values between 18°C and 190°C. The values of McCoubrey and Singh were in close agreement to the values reported in this study with less than 3% deviation through the whole temperature range. The values of Ellis and Raw were lower than the values reported in this study by as much as 7%.

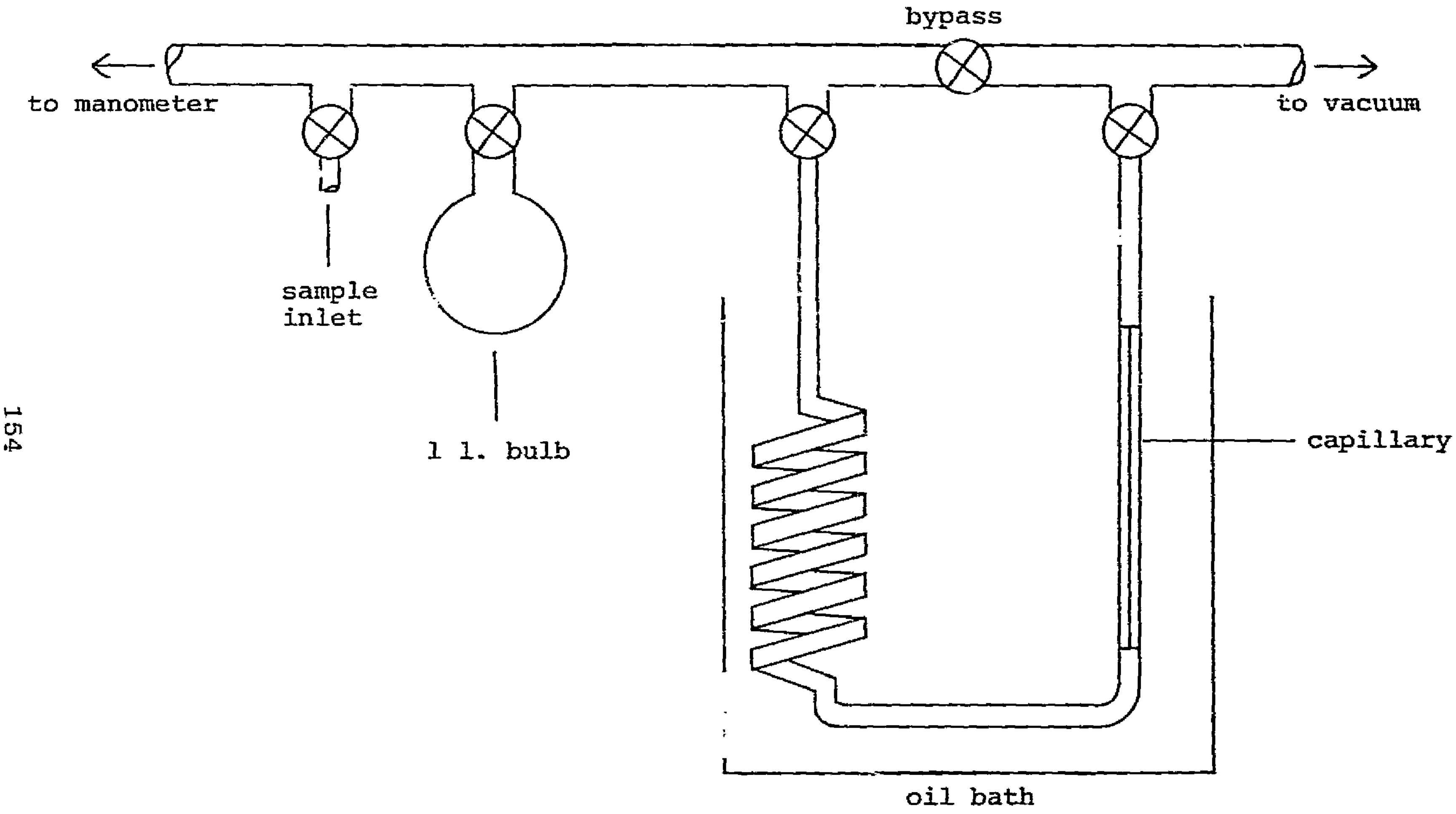

Figure 2.8-1 Constant Volume Gas Viscometer

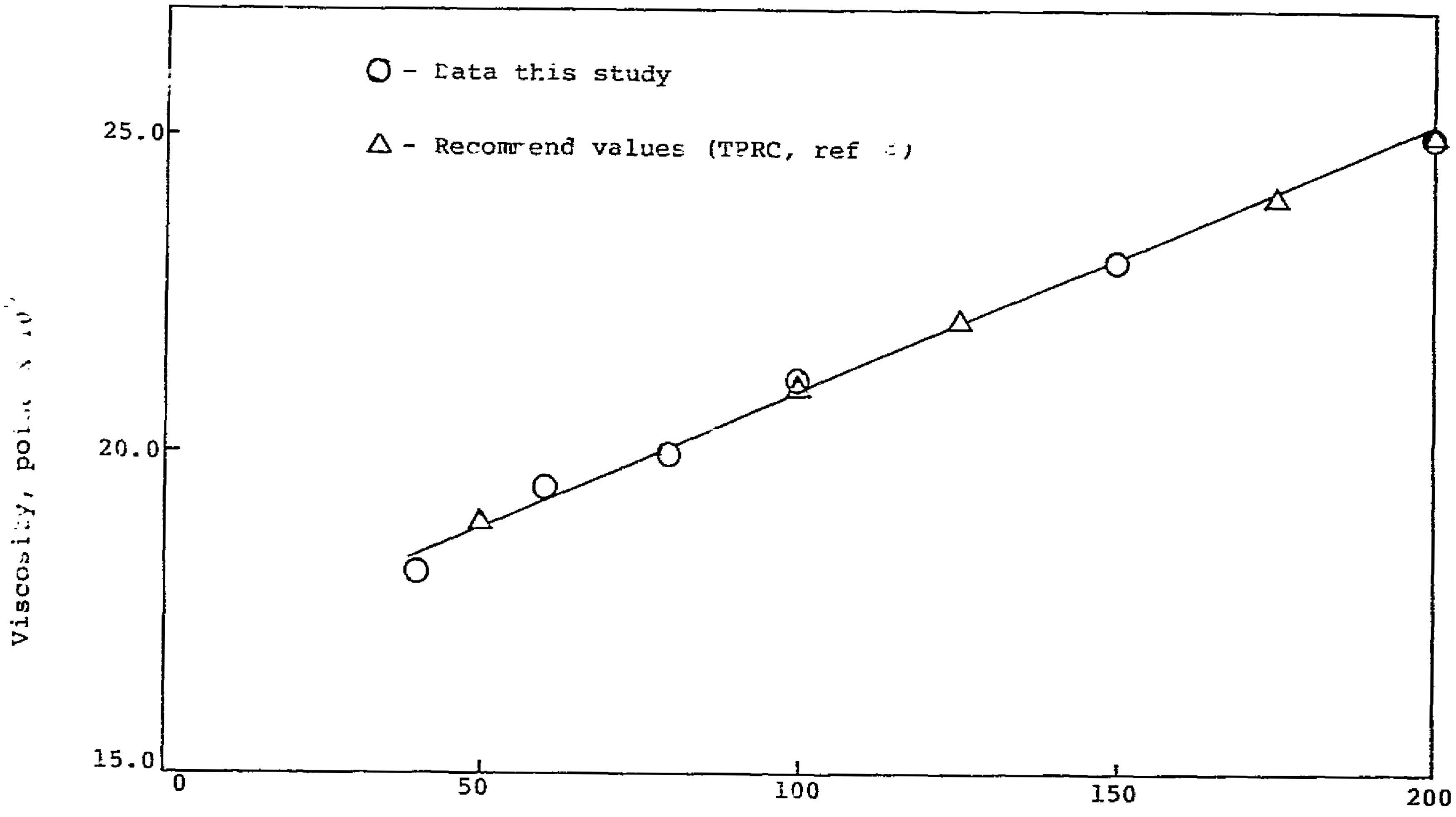

Figure 2.8-2 Viscosity of Nitrogen

Table 2.8-1

Viscosity of Gaseous Trichlorosilane

Temperature °C	Viscosity micropoise	Viscosity Nsm^{-1}	Viscosity $lb_m s^{-1} ft^{-1}$
50	122.0	12.20×10^{-6}	8.20×10^{-6}
60	125.9	12.59×10^{-6}	8.46×10^{-6}
80	134.8	13.48×10^{-6}	9.06×10^{-6}
100	140.8	14.08×10^{-6}	9.46×10^{-6}
150	157.3	15.73×10^{-6}	10.57×10^{-6}
200	177.2	17.72×10^{-6}	11.91×10^{-6}

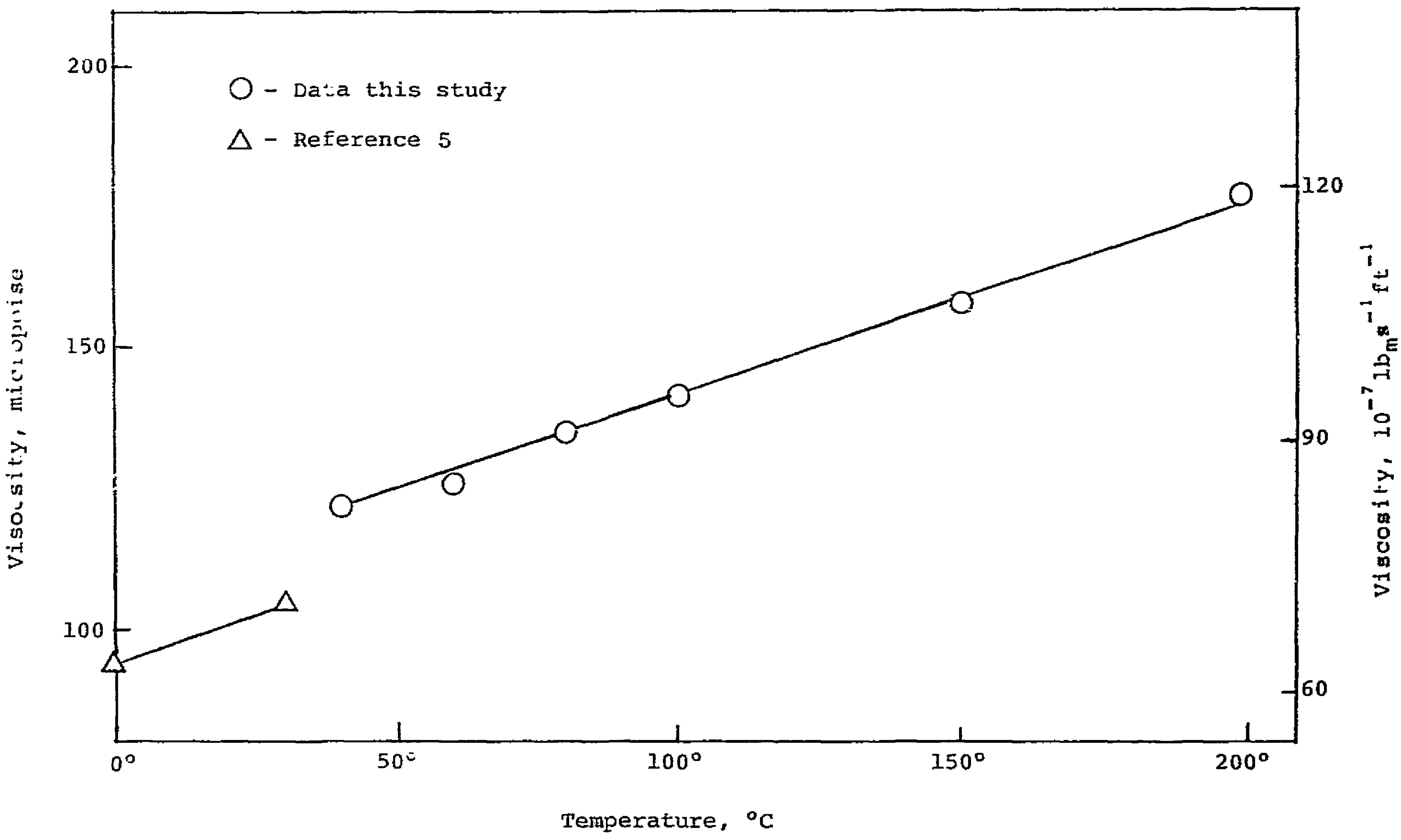

Figure 2.8-3 Viscosity of Gaseous Trichlorosilane

Table 2.8-2

Viscosity of Gaseous Dichlorosilane

Temperature	Viscosity		
°C	micropoise	Nsm^{-1}	$lb_m s^{-1} ft^{-1}$
40	118.7	11.87×10^{-6}	7.98×10^{-6}
60	125.3	12.53×10^{-6}	8.42×10^{-6}
80	134.6	13.46×10^{-6}	9.05×10^{-6}
100	140.2	14.02×10^{-6}	9.42×10^{-6}
150	163.5	16.35×10^{-6}	10.99×10^{-6}
200	181.9	18.19×10^{-6}	12.22×10^{-6}

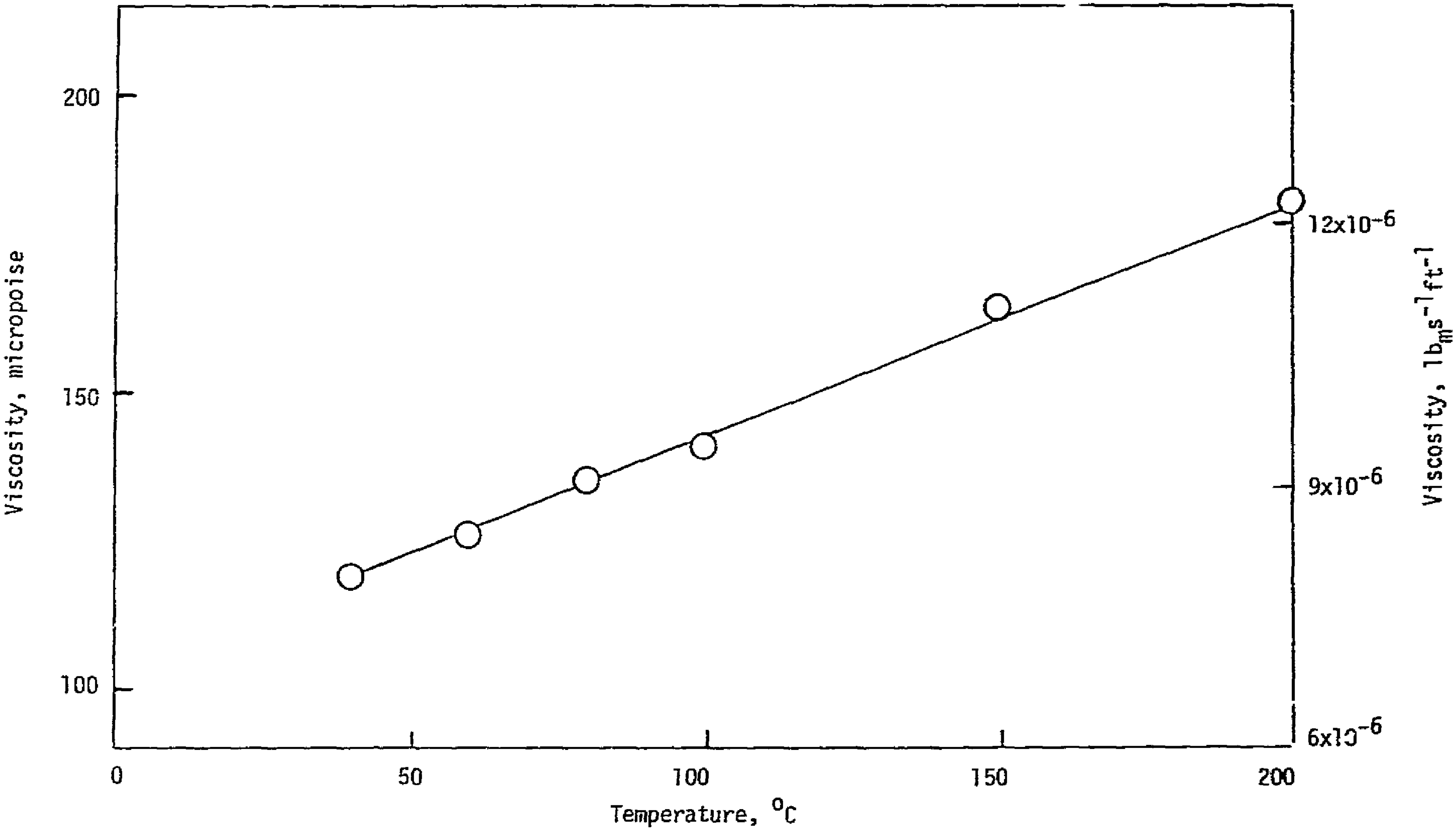

Figure 2.8-4 The Viscosity of Gaseous Dichlorosilane as a Function of Temperature

TABLE 2.8-3

Gaseous Viscosity of Tetrafluorosilane

Temperature	Viscosity		
°C	micropoise	$N\ s\ m^{-2}$	$lb_m\ s^{-1}\ ft^{-1}$
40	169.5	16.96×10^{-6}	11.40×10^{-6}
60	180.7	18.07×10^{-6}	12.14×10^{-6}
100	191.7	19.17×10^{-6}	12.88×10^{-6}
150	208.3	20.83×10^{-6}	14.00×10^{-6}
200	231.2	23.12×10^{-6}	15.54×10^{-6}

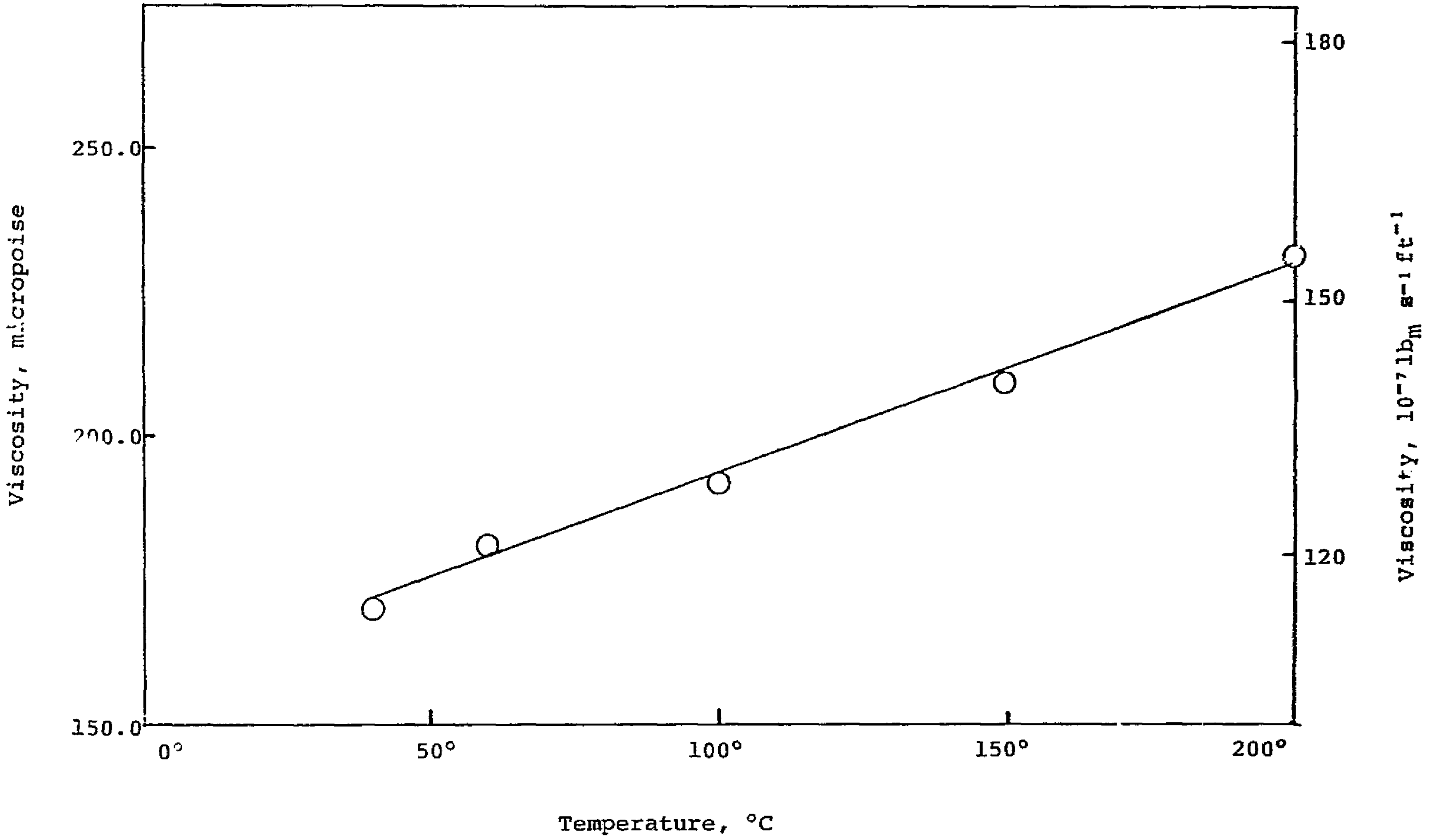

Figure 2.8-5 Viscosity of Gaseous Tetrafluorosilane

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2.9 Silicon Tetrafluoride Generation

Investigations were conducted toward developing a method to genrate silicon tetrafluoride (SiF_4) from an aqueous solution of hexafluorosilicic acid (H_2SiF_6), which is readily available as a product of the phosphate fertilizer industry. The method investigated involved the precipitation of an insoluble salt of hexafluorosilic acid followed by the thermal decomposition of the salt to produce SiF_4.

Experiments were conducted in which concentrated aqueous solutions of various salts (NaCl, NaF, NaOH, Na_2CO_3) were reacted with a 23% aqueous solution of H_2SiF_6 at room temperature:

$$2\ NaX + H_2SiF_6 \rightarrow Na_2SiF_6\downarrow + 2\ HX$$

$$\text{where } X = Cl,\ F,\ OH \text{ or } CO_3$$

Reaction under these conditions resulted in the immediate formation of a precipitate which could be readily filtered and dried. With each salt, several reactions were carried out with differing stoichiometric amounts of the reactant in order to determine the reactant ratio which would give maximum precipitation of Na_2SiF_6. The results of these investigations are shown in Figures 2.9-1 through 2.9-4.

Figure 2.9-1 shows that the precipitation of Na_2SiF_6 with NaCl solutions gives maximum recovery of the SiF_4 precursor at a reactant ratio of slightly greater than 1:1. Increasing the amount of NaCl does not improve the yield any further. The percent yield of Na_2SiF_6 never rises above the 90-95% region due to its slight solubility in water. The precipitate formed was shown to be Na_2SiF_6 by comparing its infrared spectrum with that of an authentic sample. Air drying of the precipitate was shown to leave approximately 1-2% water.

Figure 2.9-2 shows that precipitation of Na_2SiF_6 with NaF solution gives essentially the same results as was obtained with NaCl up to about 1.25:1 reactant ratio. At higher ratios the calculated percent yield of Na_2SiF_6 rises above 100% which indicates that something else is occurring other than the precipitation of Na_2SiF_6. Hydrofluoric acid (HF) is a byproduct of this reaction and will form an insoluble adduct (NaF·HF) which results in the greater than 100% calculated yield.

Precipitation using NaOH solutions (Figure 2.9-3) gives completely different results than that obtained with either NaCl and NaF. The calculated yields (based on Na_2SiF_6) are much above 100% and continue to rise up to a reactant ratio of 3:1. The use of NaOH (a strongly basic reagent) resulted in the hydrolysis of the Si-F bond as well as precipitation of Na_2SiF_6. The hydrolysis of $SiF_6^=$ under basic conditions results in the formation of silicic acids which are hydrated oxides of silicon and these precipitate along with Na_2SiF_6. The formation of silicic acids in these reactions was confirmed by infrared analysis of the precipitate which showed characteristic absorptions for both silicic acid and Na_2SiF_6.

Figure 2.9-4 shows that reaction with Na_2CO_3 (a weakly basic reagent) gives results comparable to those obtained with NaCl solutions. Infrared analysis of the precipitate however, indicated the presence of some silicic acids which showed that hydrolysis was occurring with Na_2CO_3 as well as with NaOH.

Studies were also conducted to determine conditions necessary for the efficient precipitation of $BaSiF_6$ (another possible precursor for the geration of SiF_4). The use of $BaSiF_6$ as an alternate precursor to SiF_4 (instead of Na_2SiF_6) was investigated because of several advantages this route may have. $BaSiF_6$ is less soluble than Na_2SiF_6 by a factor of about 30 which should result in a more efficient recovery of SiF_4 from a solution of H_2SiF_6. Secondly, if BaF_2 is used to precipitate the $BaSiF_6$ there should be no co-precipitation of an adduct with HF (use of NaF in the precipitation of Na_2SiF_6 resulted in the co-precipitation of NaF•HF). Also the thermal decomposition of $BaSiF_6$ to give SiF_4 may occur at a lower temperature than that observed for Na_2SiF_6.

The precipitation of $BaSiF_6$ was effected by the reaction of a 23% aqueous solution of H_2SiF_6 with aqueous solutions of either $BaCl_2$ or BaF_2. An immediate precipitate was formed in both

$$BaX_2 + H_2SiF_6 \rightarrow BaSiF_6\downarrow + 2\ HX$$

$$X = Cl,\ F$$

cases which could be readily filtered and dried. With each salt, several reactions were carried out with differing stoichiometric amounts of the reactant in order to determine the reactant ratio which would give maximum precipitation of $BaSiF_4$. The results of these investigations are presented in Figures 2.9-5 and 2.9-6.

Figure 2.9-5 shows that the precipitation of $BaSiF_6$ with $BaCl_2$ solutions at room temperature gives maximum recovery of the SiF_4 precursor at a reactant ratio of 1:1. Increasing the amount of $BaCl_2$ does not increase the yield any further and the percent yield never rises above about 97% due to the slight solubility of $BaSiF_6$.

Figure 2.9-6 shows the results of the reactions of BaF_2 solutions with H_2SiF_6 at 60°C. Maximum recovery of $BaSiF_6$ is shown to be at a reactant ratio of 1.5 to 1 with the percent yield about 95%. The higher reactant ratio necessary for efficient precipitation and slightly lower yields than were observed in the reactions with $BaCl_2$ is due to the low solubility of BaF_2 which dictated the use of considerably larger volumes of water.

Investigations were conducted for the generation of silicon tetrafluoride (SiF_4) by the thermal decomposition of sodium hexafluorosilicate (Na_2SiF_6):

$$Na_2SiF_6 \overset{\Delta}{\rightleftarrows} SiF_4\uparrow + 2\ NaF \qquad (4)$$

Parameters such as temperature, reaction time, and general reaction conditions were examined in order to determine optimum conditions for efficient SiF_4 generation.

Anhydrous sample of Na_2SiF_6 were placed in a quartz tube and heated under various reaction conditions. The amount of SiF_4 generated was determined from the weight loss of the sample after heating based on the stoichiometry in equation 4.

Initially the samples were heated for 1 hour in a closed system of inert gas (N_2) maintained at 1 atmosphere and at constant temperatures ranging from 350°C to 600°C. In no instance was the generation of SiF_4 above 12%. This low yield of the SiF_4 was due to the fact that the thermal decomposition reaction is an equilibrium reaction (eq. 4) and when the decomposition is carried out under conditions which allow an equilibrium to be established, the reaction will proceed no further than the equilibrium point.

As a result of these initial results, the reaction conditions were altered such that a slow stream of N_2 (approximately 200 cc/min) was continuously passed over the sample during the decomposition. Figure 2.9-7 shows the results of these experiments. Heating the samples for 1 hour gave low yields of SiF_4 increased rapidly such that the generation of SiF_4 was essentially quantitative above 550°C.

Based on the above results, it is obvious that the decomposition of Na_2SiF_6 to generate SiF_4 occurs extensively at temperatures above 500°C. Since this data was obtained by heating the samples for an extended period (1 hour at each temperature), the per cent generation of SiF_4 was obtained as a function of reaction time in order to determine the minimum amount of heating required to produce high yields of SiF_4. Figures 2.9-8, 2.9-9, 2,9-10 show the results of this type investigation at 500°C, 550°C, and 600°C. Figure 2.9-8 indicates that decomposition is not complete at 500°C even upon heating for a period of 1 hour. At 550°C the generation of SiF_4 approaches completion in 30 minutes (figure 2.9-9) and at 600°C the reaction is essentially complete in 15 minutes.

The generation of silicon tetrafluoride (SiF_4) by the thermal decomposition of barium hexafluorosilicate ($BaSiF_6$) according to equation 9 was investigated. Parameters such

$$BaSiF_6 \overset{\Delta}{\rightleftarrows} SiF_4\uparrow + BaF_2 \qquad (9)$$

as temperature, reaction time, and general reaction conditions were examined in order to determine optimum conditions for efficient SiF_4 generation by this method.

Samples of anhydrous $BaSiF_6$ were placed in a quartz tube and heated at various temperatures for a period of one hour during which time a slow stream of N_2 (approximately 200 cc/min) was continuously passed over the sample. The amount of SiF_4 generated was determined from the weight loss of the sample after heating based on the stoichiometry in equation 9. The results of these experiments are shown in figure 2.9-11. Heating for 1 hour at temperatures up to about 400°C gave low yields of SiF_4. At temperatures above 400°C however, nearly quantitative yields were obtained.

Based on the above results, it can be seen that the decomposition of $BaSiF_6$ to generate SiF_4 occurs extensively at temperatures above 400°C. Since this data was obtained by heating the samples for an extended period (1 hour at each temperature), the per cent yield of SiF_4 was obtained as a function of time in order to determine the minimum amount of heating required to produce high yields of SiF_4. Figures 2.9-12, 2.9-13, 2.9-14, 2.9-15 show the results of this type investigation at 400°C, 450°C, 500°C, and 550°C respectively. Figure 2.9-12 shows that at 400°C the decomposition of $BaSiF_6$ does not approach completion until about 1 hour heating time. Figure 2.9-13 shows that decomposition of $BaSiF_6$ is essentially complete after 30 minutes heating at 450°C and figures 2.9-14 & 2.9-15 show that decomposition is complete after only a few minutes (5-10 minutes) at 500°C and 550°C.

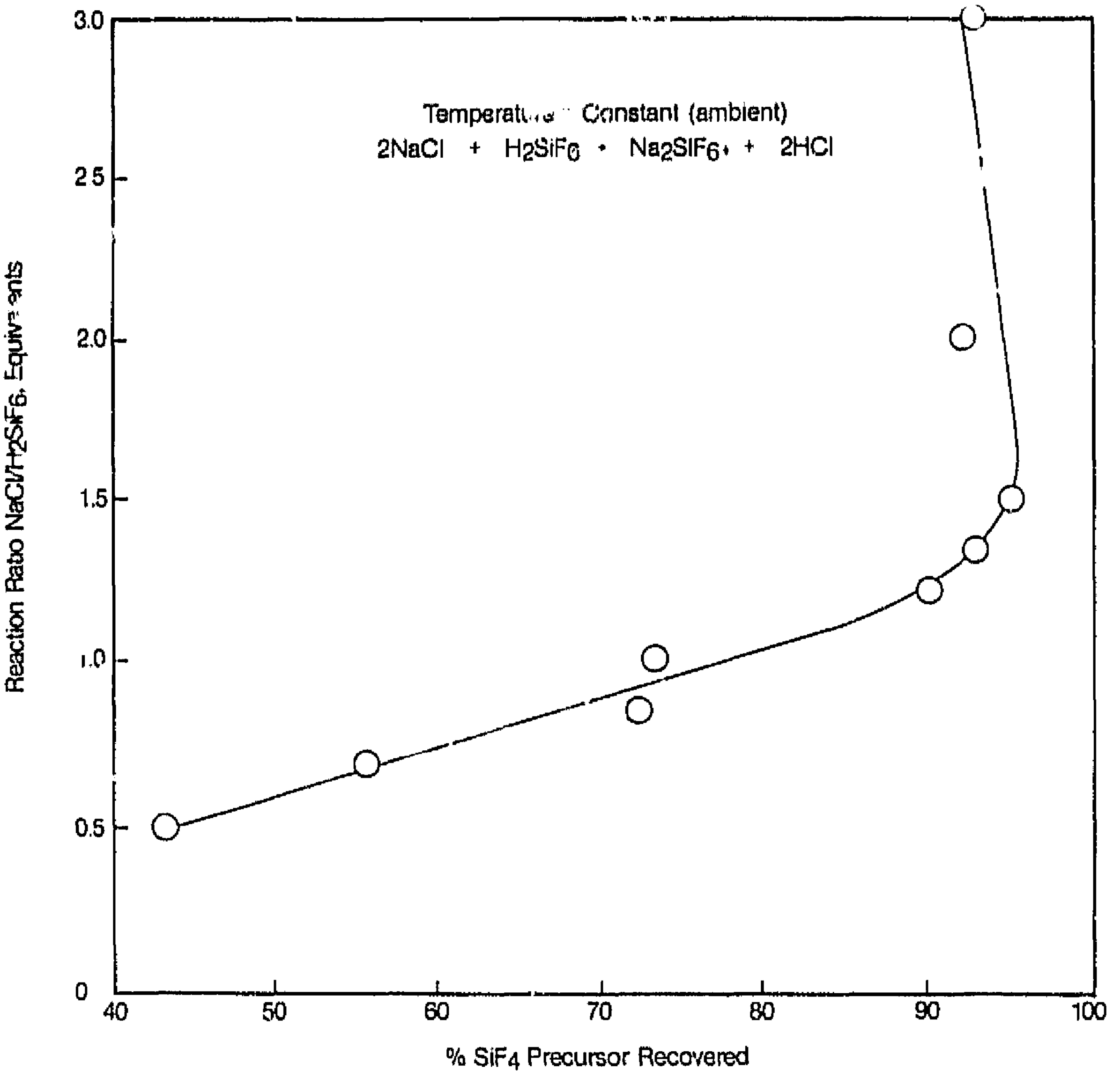

Figure 2.9-1 Variation of SiF_4 Precursor Recovery with Reaction Ratio (NaCl Reaction)

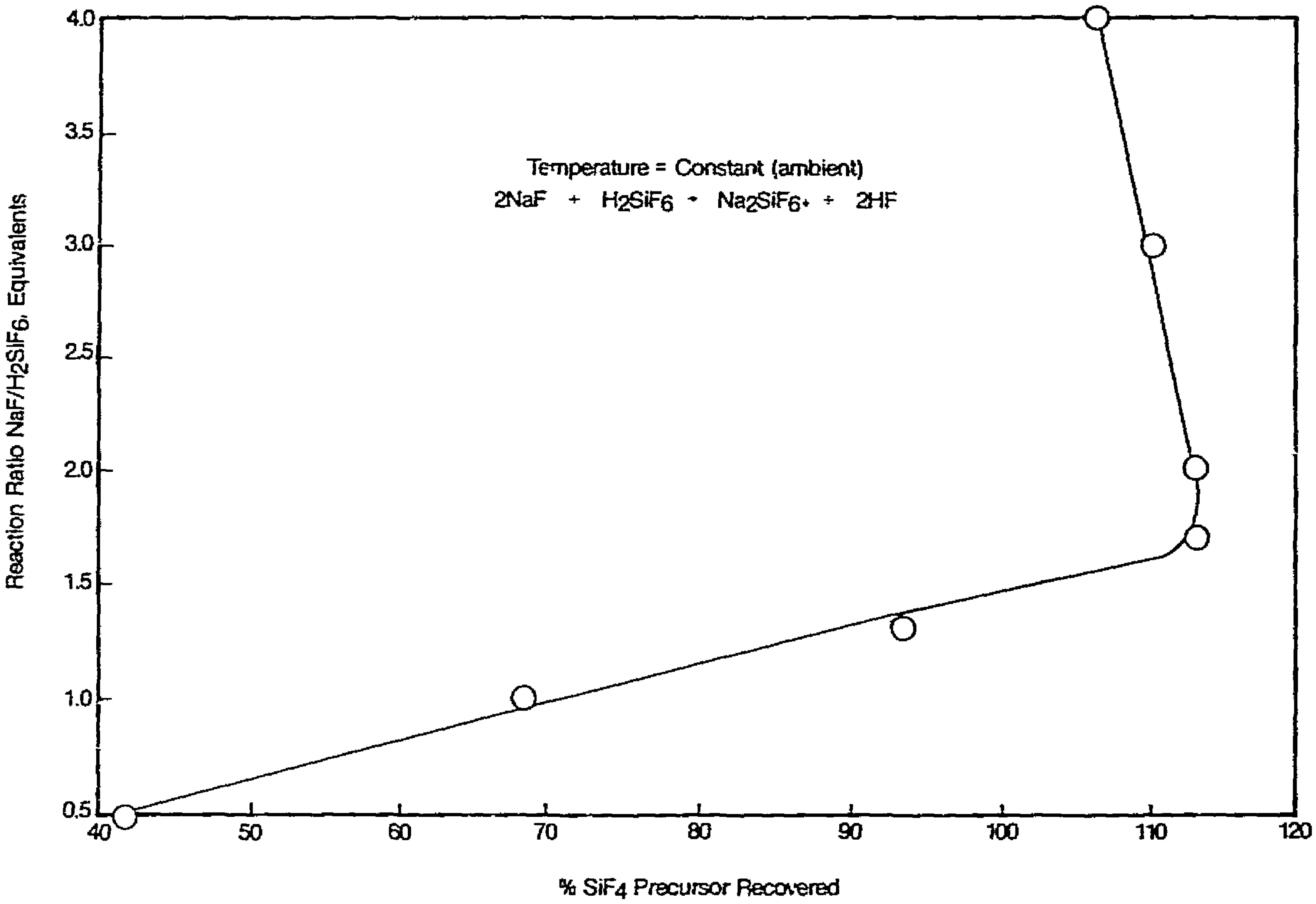

Figure 2.9-2 Variation of SiF_4 Precursor Recovery with Reaction Ratio (NaF Reaction)

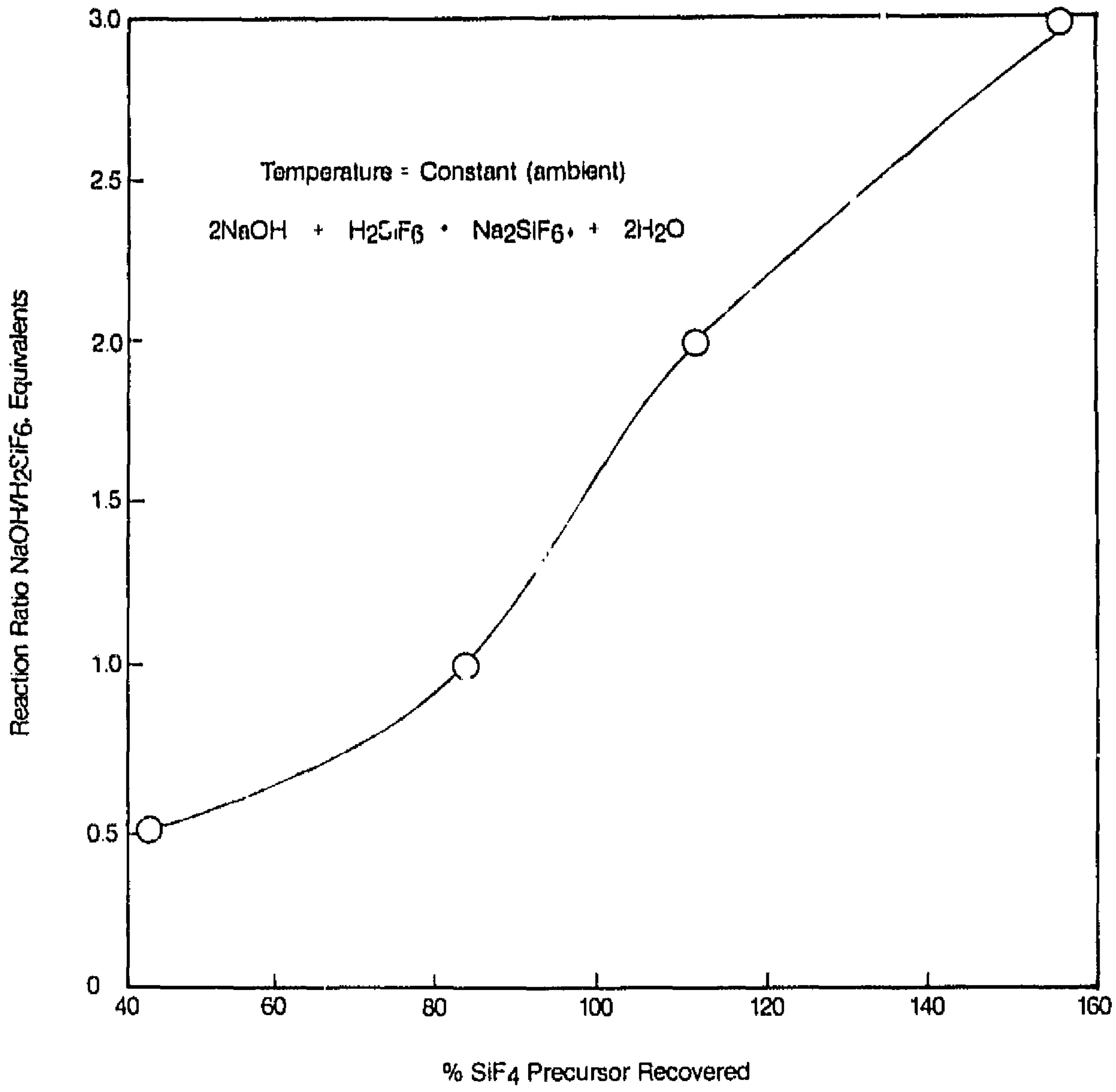

Figure 2.9-3 Variation of SiF_4 Precursor Recovery with Reaction Ratio (NaOH Reaction)

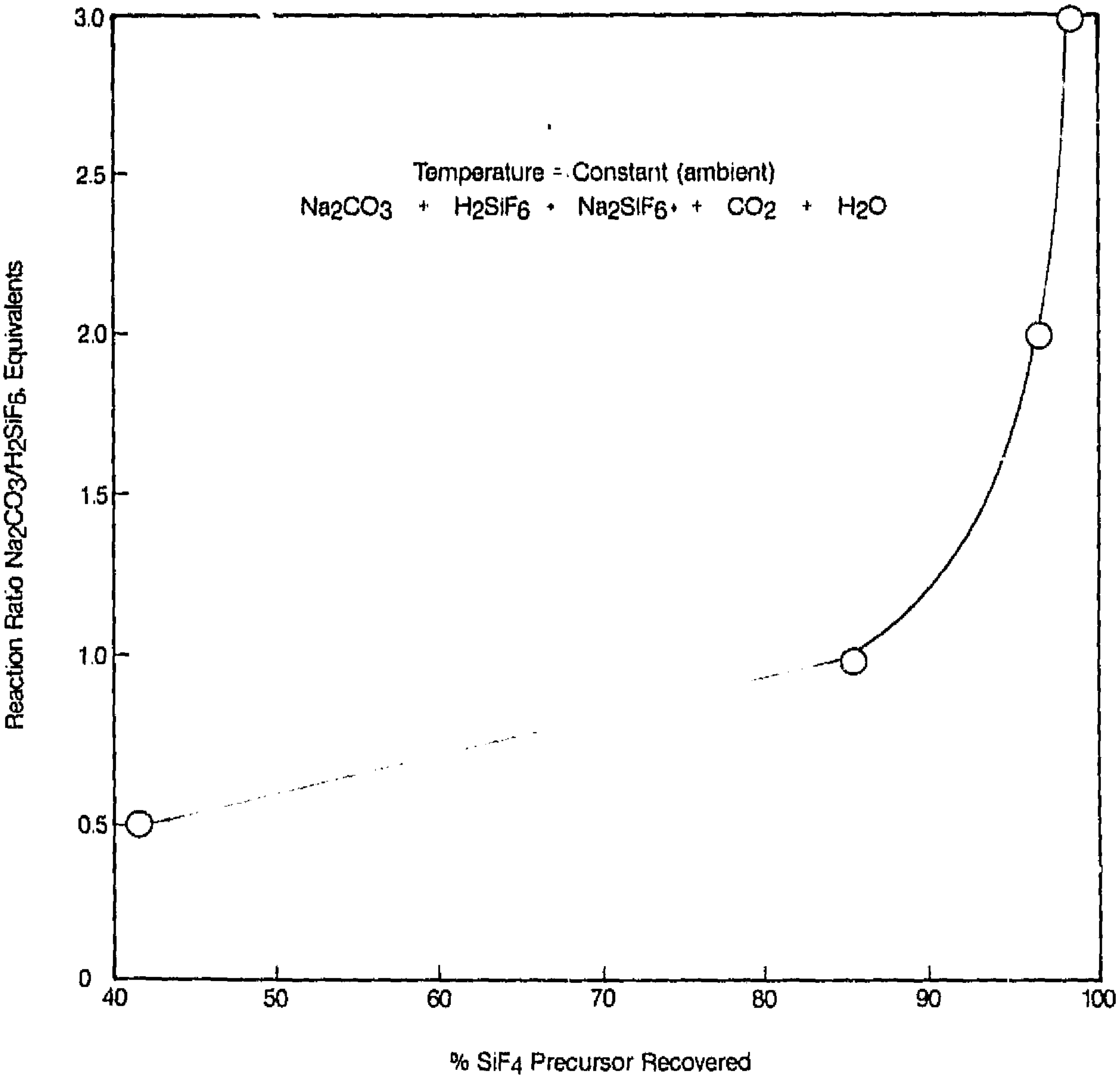

Figure 2.9-4 Variation of SiF_4 Precursor Recovery with Reaction Ratio (Na_2CO_3 Reaction)

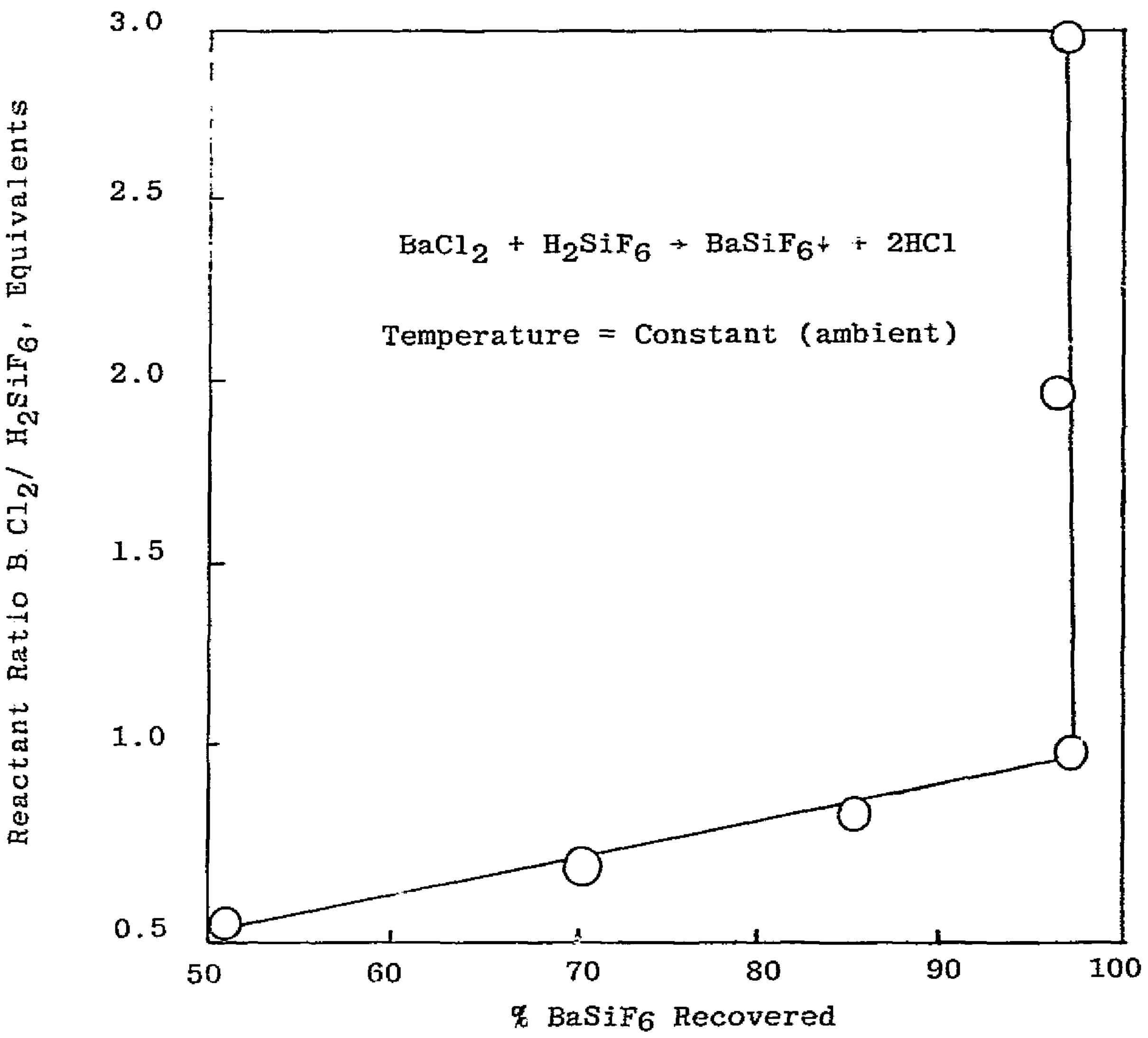

Figure 2.9-5 Variation of $BaSiF_6$ Recovery with Reactant Ratio ($BaCl_2$ Reaction)

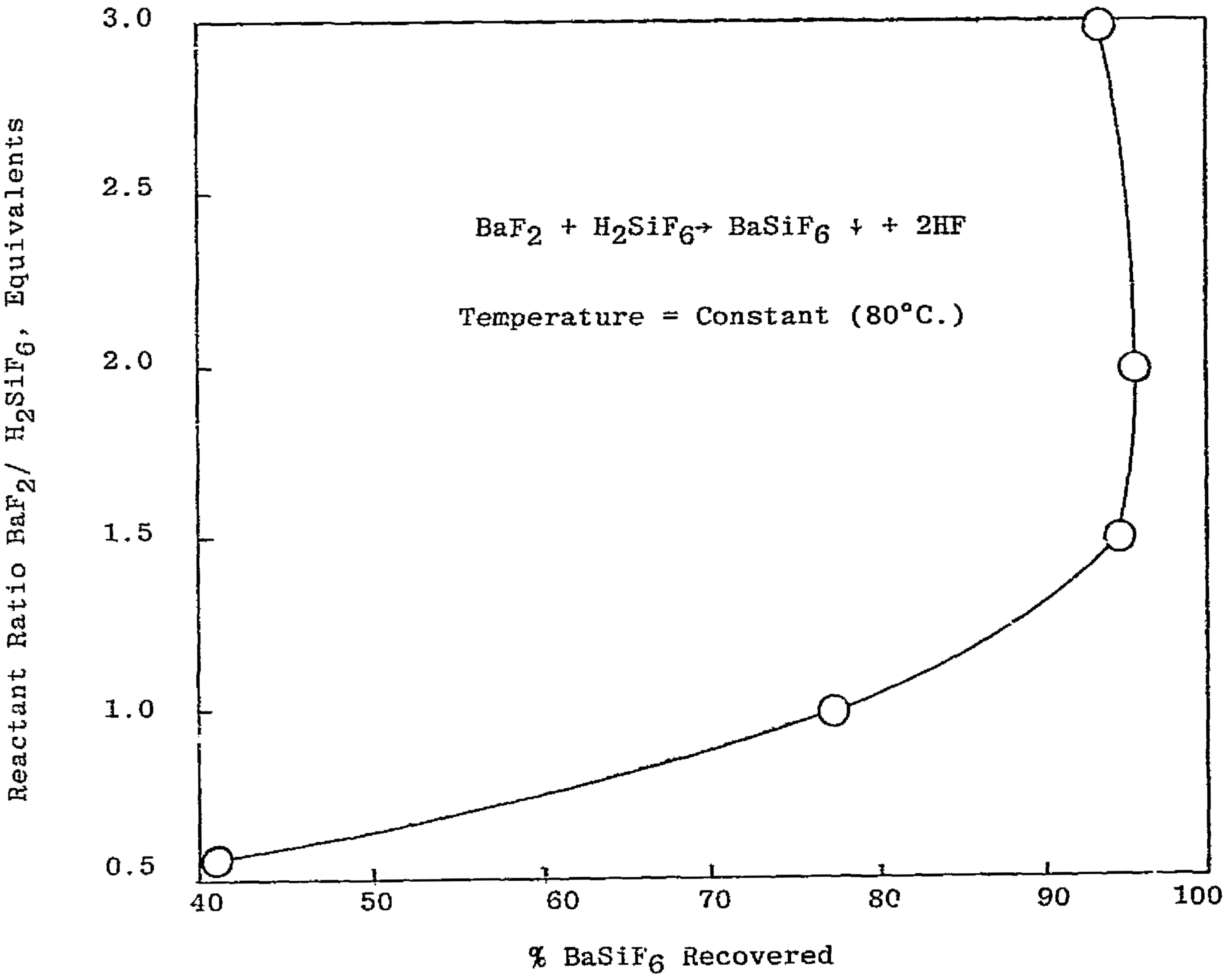

Figure [illegible] Variation of $BaSiF_6$ Recovery with Reactant Ratio (BaF [illegible]

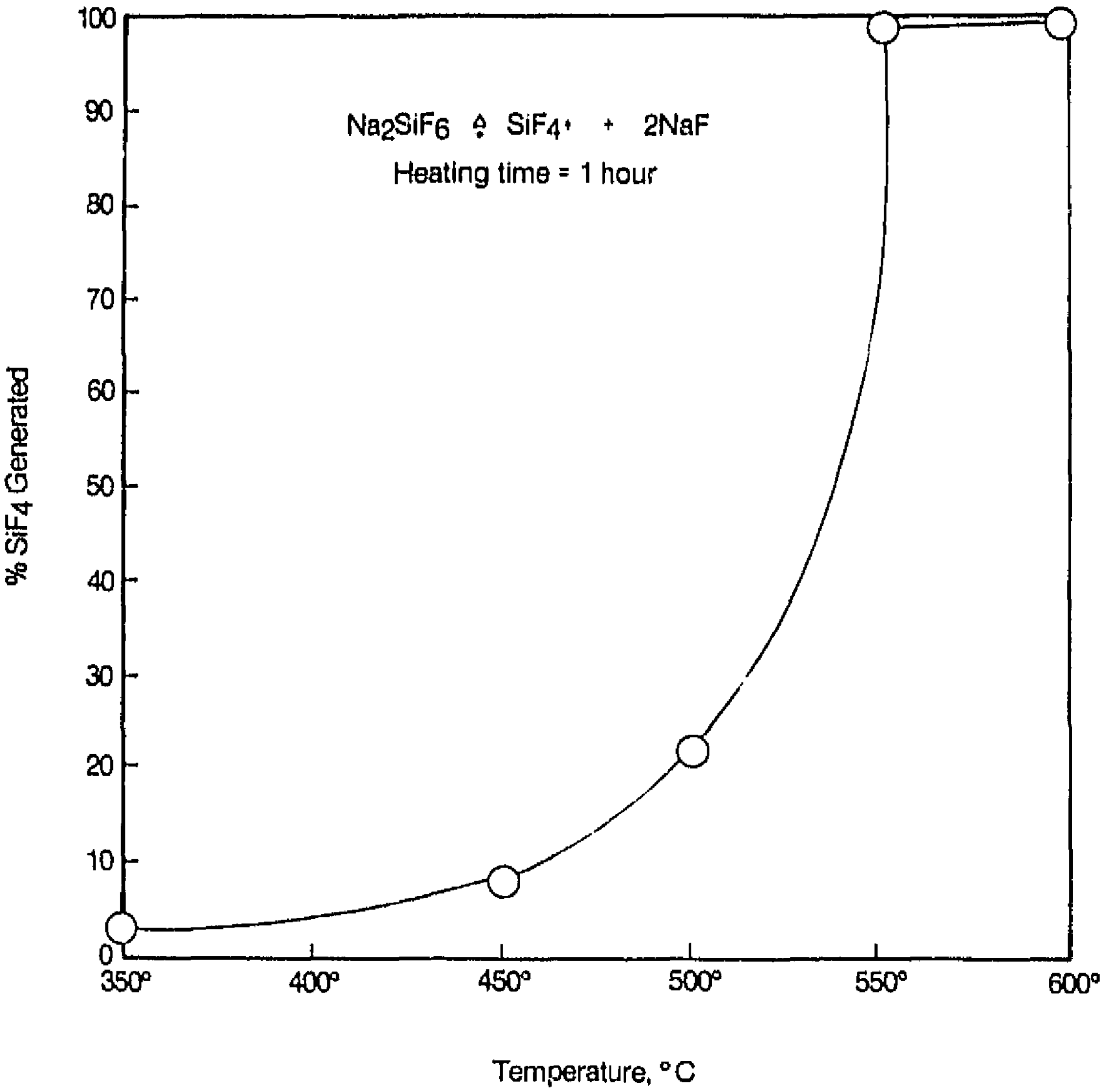

Figure 2.9-7 Variation of % SiF_4 Generated with Temperature

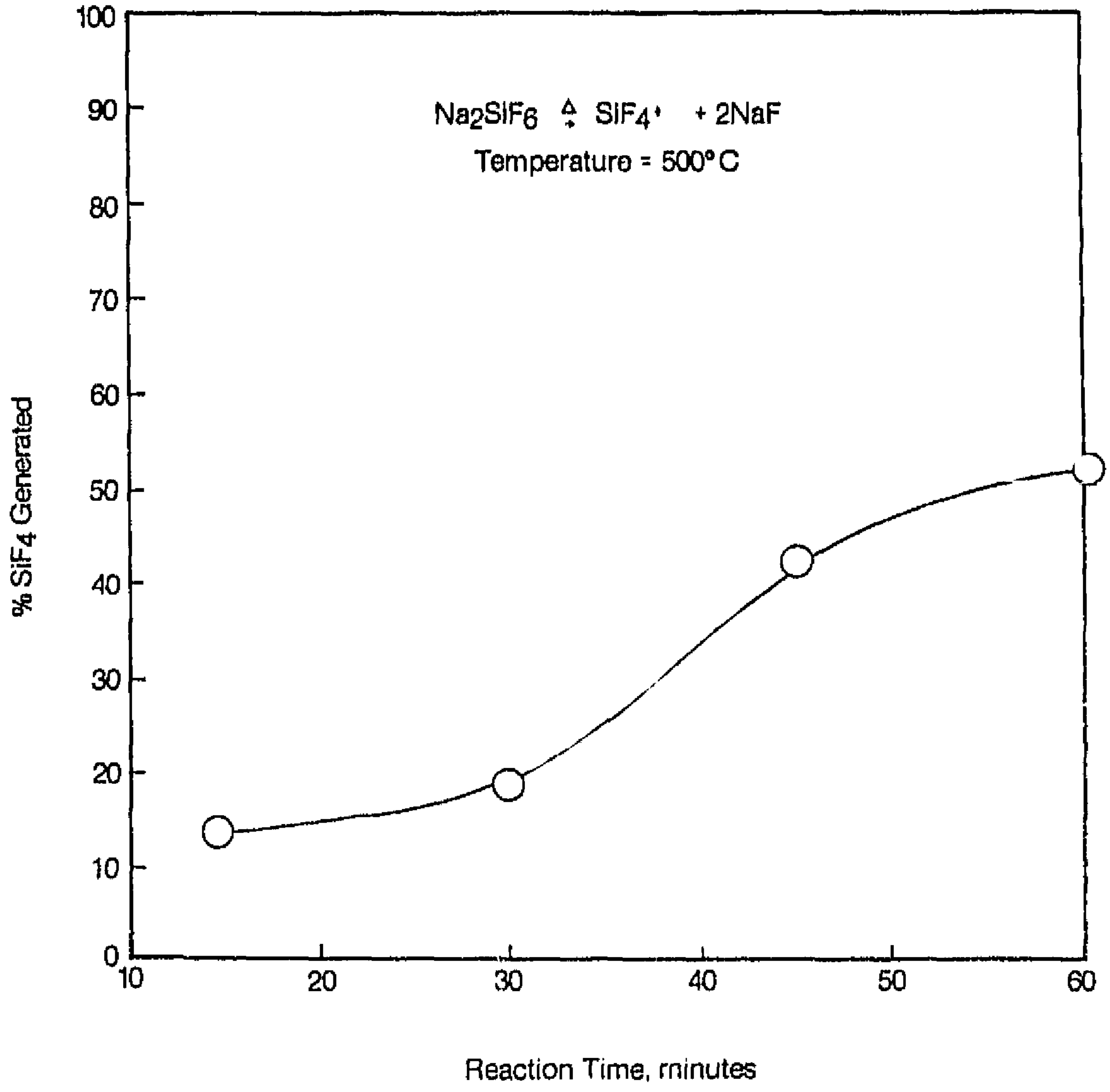

Figure 2.9-8 Variation of % SiF_4 Generated with Reaction Time

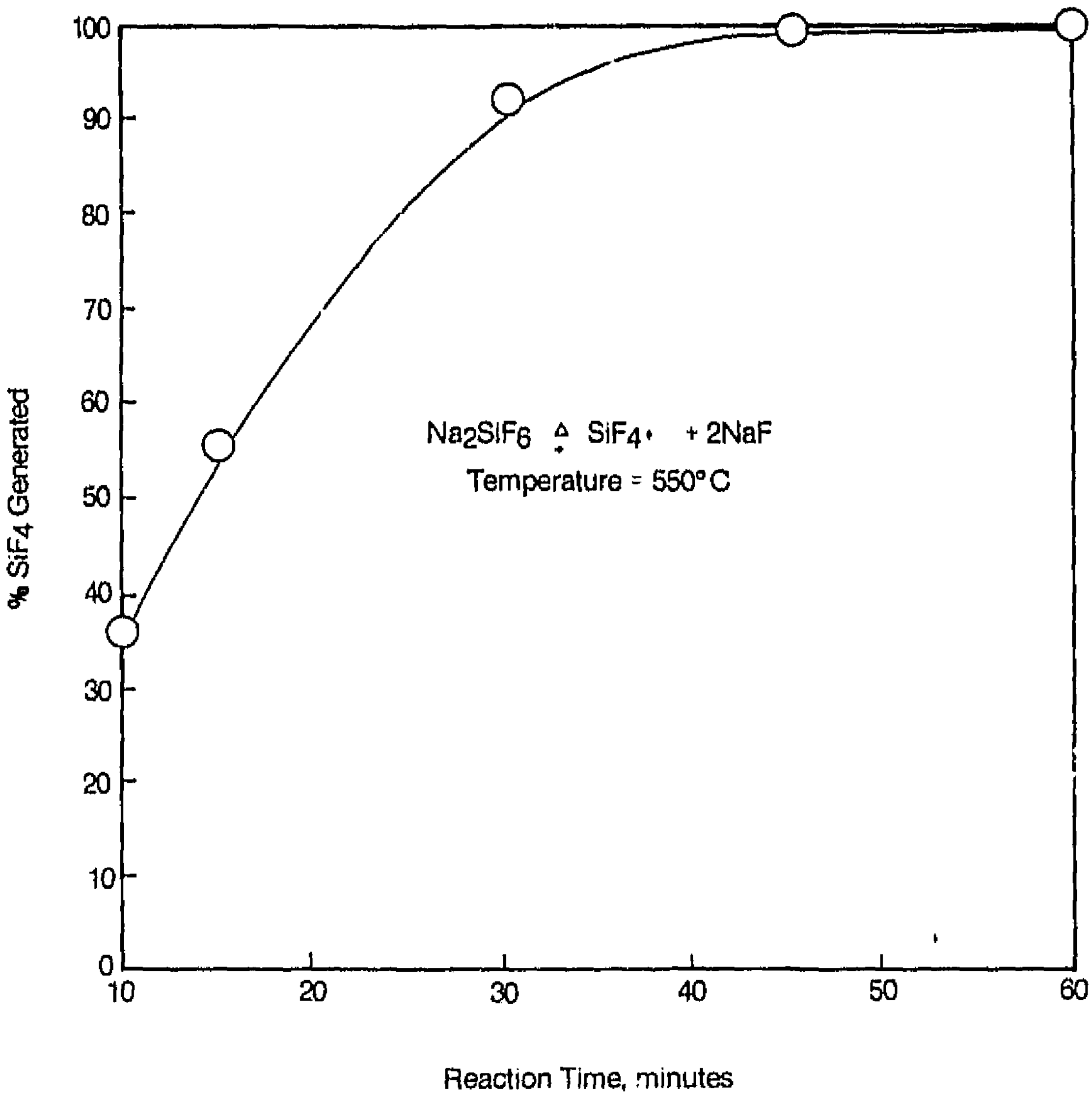

Figure 2.9-9 Variation of % SiF_4 Generated with Reaction Time

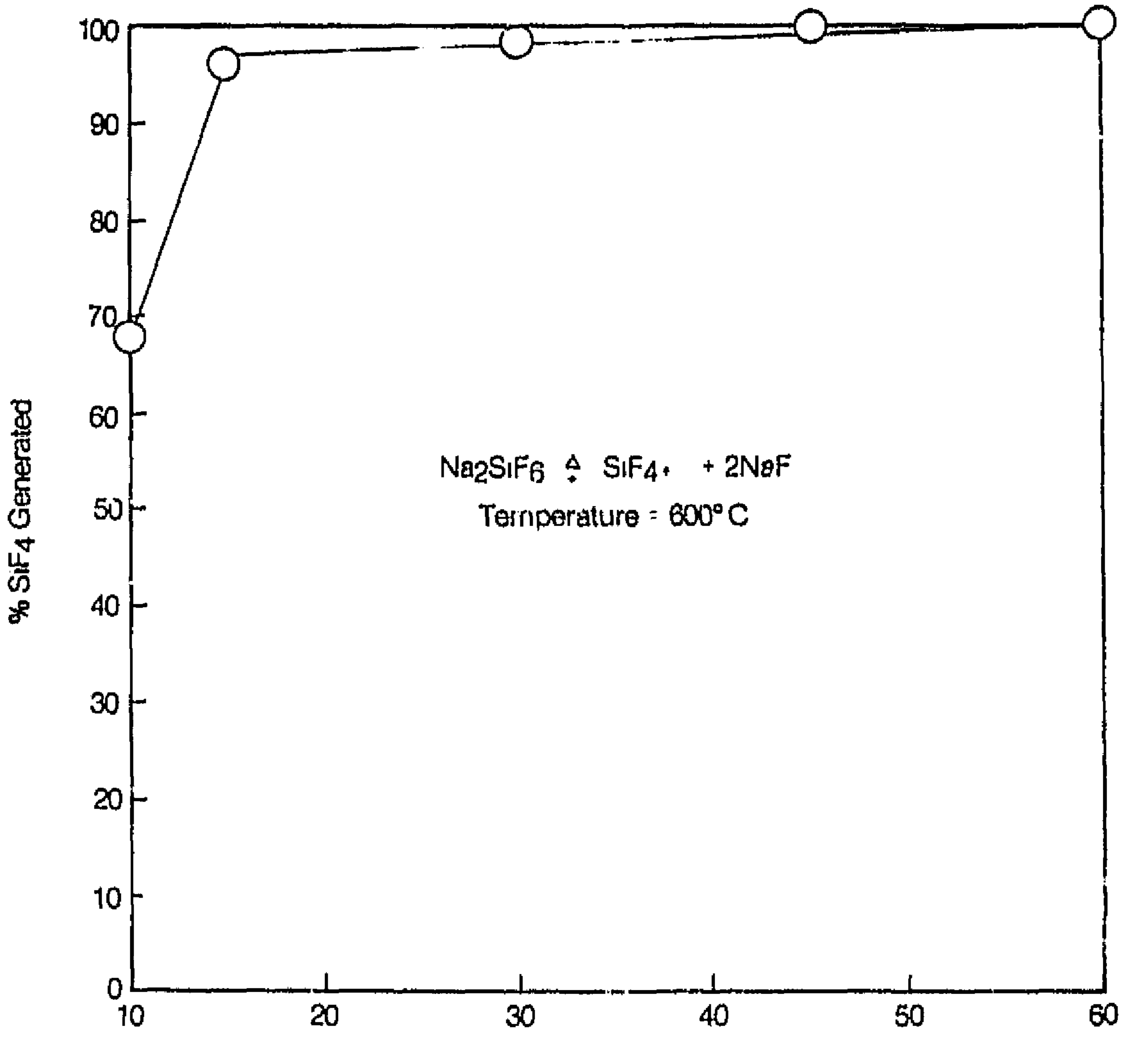

Figure 2.9-10 Variation of % SiF_4 Generated with Reaction Time

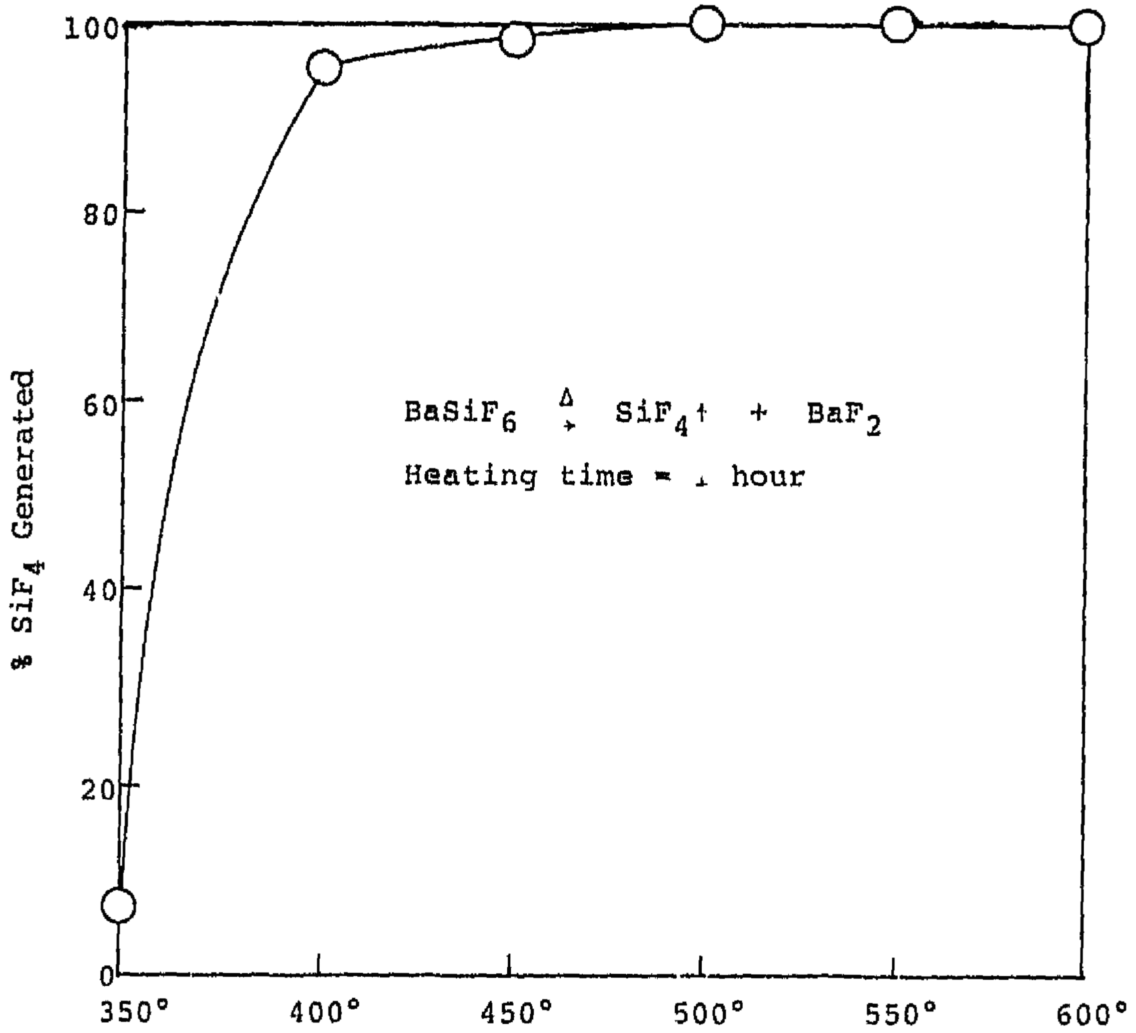

Figure 2.9-11 Variation of % SiF_4 Generated with Temperature

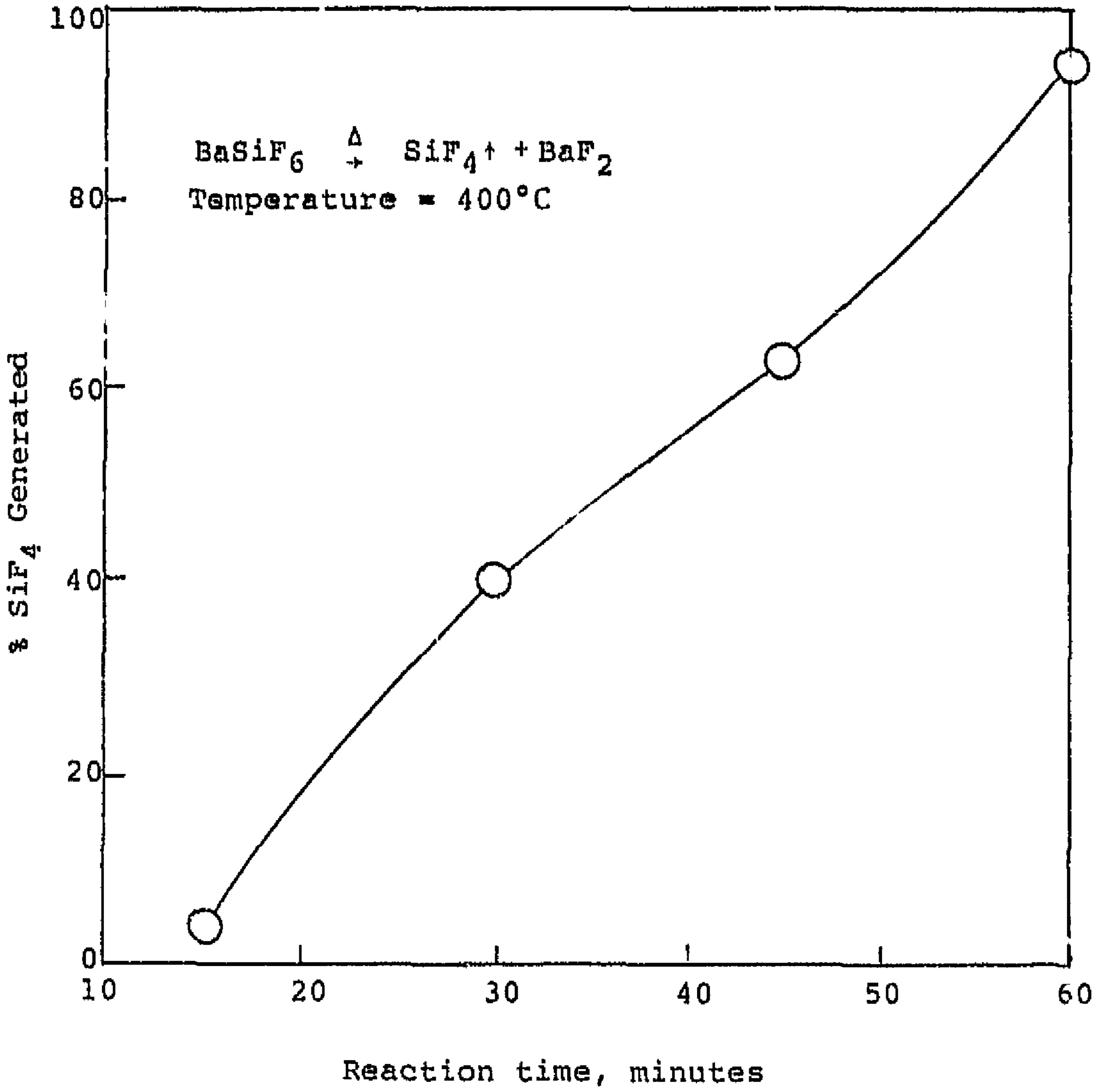

Figure 2.9-12 Variation of % SiF_4 Generated with Reaction Time

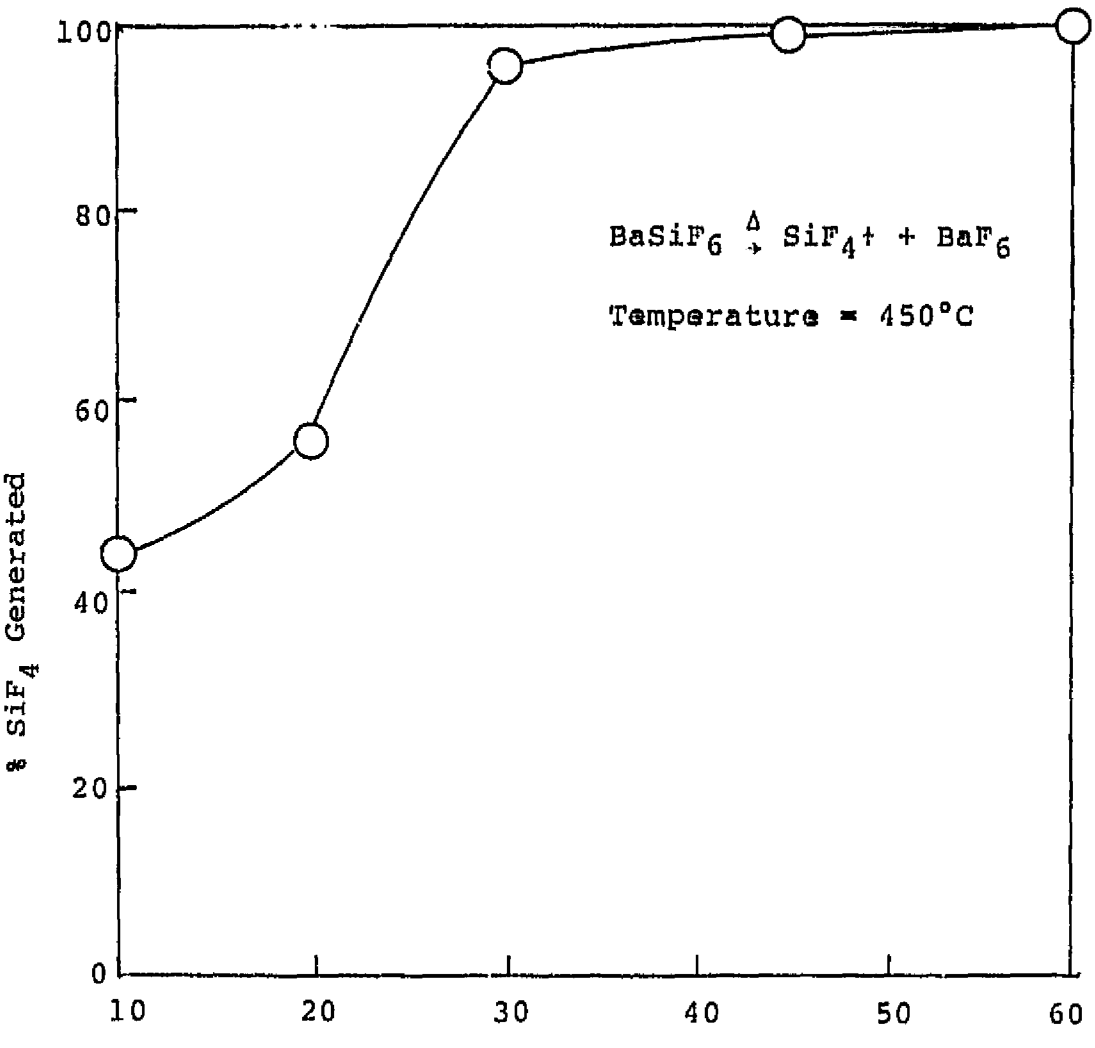

Figure 2.9-13 Variation of % SiF_4 Generated with Reaction Time

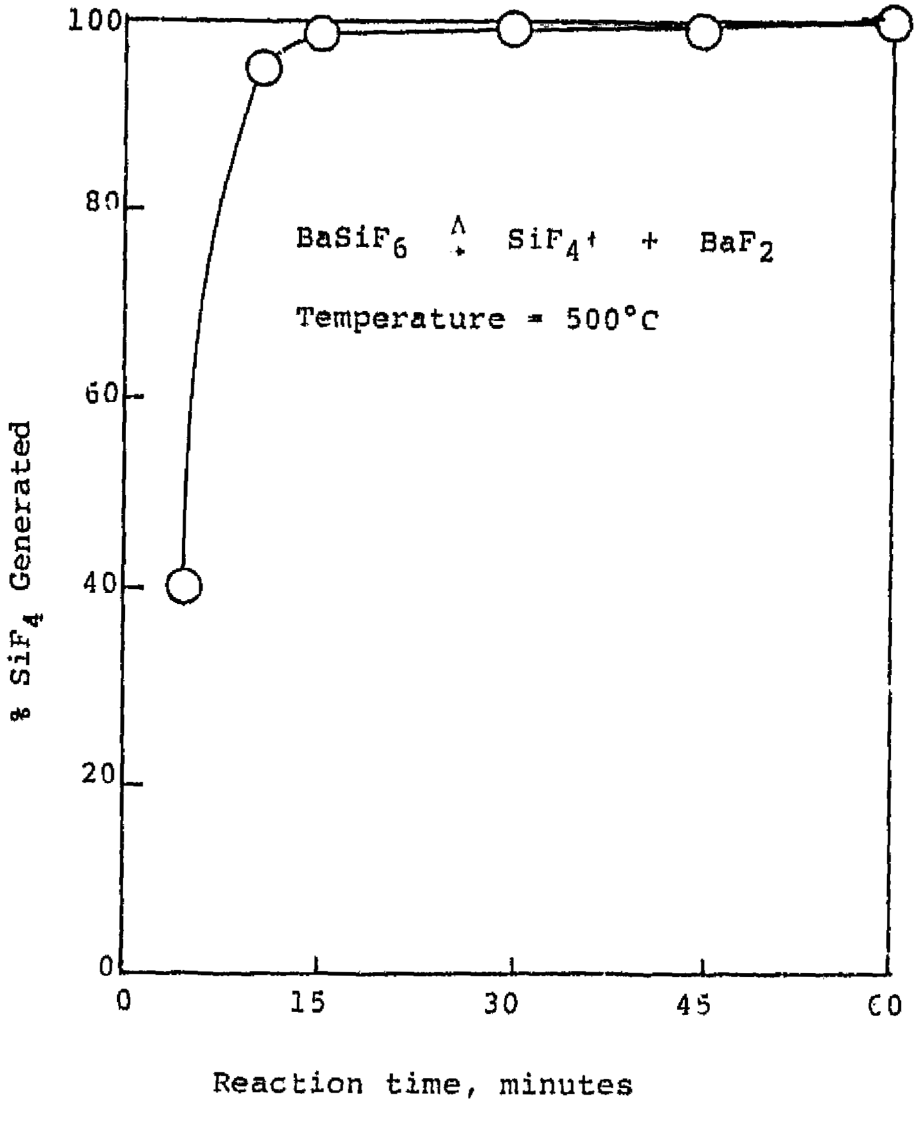

Figure 2.9-14 Variation of % SiF_4 Generated with Reaction Time

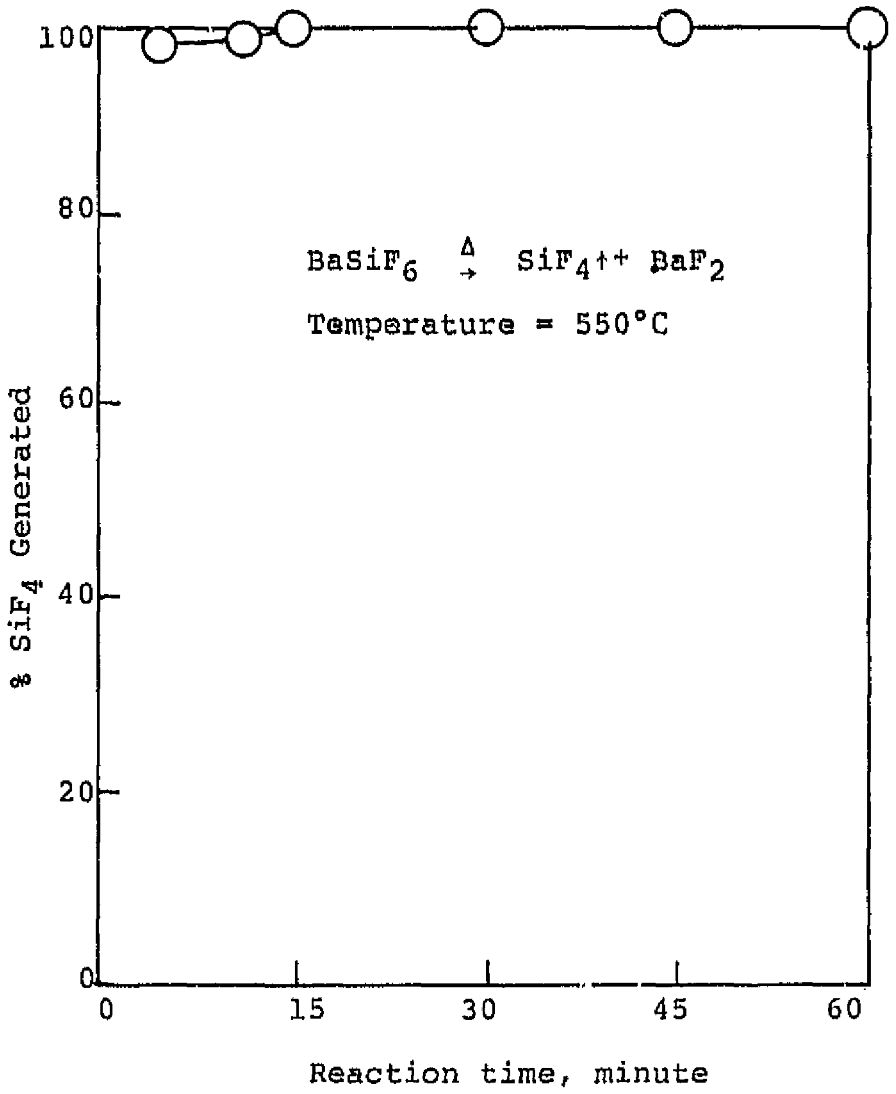

Figure 2.9-15 Variation of % SiF_4 Generated with Reaction Time

3. CHEMICAL ENGINEERING ANALYSES

3.1 SiI_4 Decomposition Process

The chemical engineering analysis activity involves a preliminary process design of a plant to produce silicon via the technology under consideration.

The process flow-diagram for the SiI_4 decomposition process is shown in Figure 3.1-1. This process involves several major processing operations such as fluidization, distillation, condensation, vaporization and deposition unit.

At the beginning of the process, metallurgical grade silicon (M.G. Si) is reacted with iodine (I_2) in a fluidized bed reactor (100°K) to produce silicon tetraiodide. This gas product is condensed and then purified by distillation process.

This purified SiI_4 is vaporized and introduced into a silicon rod reactor where silicon is deposed according to the following reaction

$$SiI_4 \longrightarrow Si + 2I_2 \qquad (3.1\text{-}1)$$

The reaction temperature is kept at 1300°K.

Unreacted SiI_4 and iodine are condensed and separated by distillation for recycle purpose.

A process design was performed to obtain data for the cost analysis. The design was based on a plant for the production of 1000 metric tons per year of polysilicon via this SiI_4 decomposition process.

The detailed status sheet for the process design package is shown in Table 3.1-1 and is representative of the various sub-items that make up the activity. 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

Base Case Conditions------------	Table 3.1-2
Reaction chemistry-----------------	Table 3.1-3
Raw Material Requirements------	Table 3.1-4
Utility Requirements-------------	Table 3.1-5
Major Process Equipment---------	Table 3.1-6
Production Labor Requirements-	Table 3.1-7

The process design provides detailed data for raw materials, utilities, major process equipment and production labor requirements which are necessary for polysilicon production

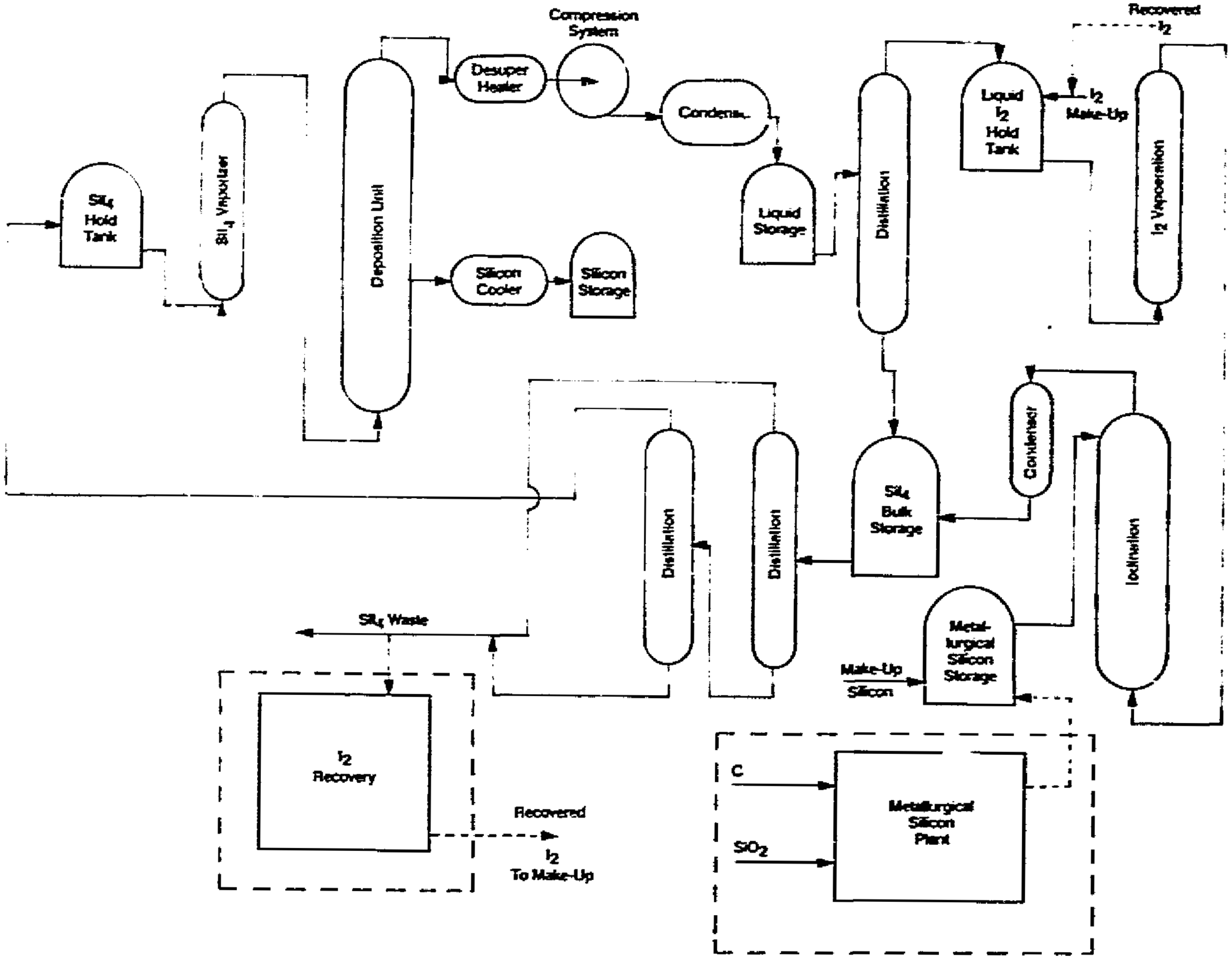

Figure 3.1-1 Process Flow Diagram for SiI$_4$ Decomposition Process (Battelle)

TABLE 3.1-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR SiI_4 DECOMPOSITION PROCESS

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

○ Plan
◐ In Progress
● Complete

TABLE 3.1-2

BASE CASE CONDITIONS FOR SiI_4 DECOMPOSITION PROCESS

1. Plant Size
   - Production of 1000 metric tons/year
   - Solar Cell Grade Silicon

2. Iodination Reaction
   - Metallurgical grade silicon and iodine to produce SiI_4
   - Atmospheric, 1000°K
   - 100% conversion (thermodynamic equilibrium)
   - Fluidized bed

3. SiI_4 Purification
   - Recycled and manufactured SiI_4 distilled
   - 10% waste (5% light, 5% heavies)
   - 90% product (heartcut)

4. SiI_4 Decomposition
   - Silicon rod reactor, deposition
   - .001 ATM, 1300°K
   - 59.67% conversion (thermodynamic equilibrium)

5. SiI_4/I_2 Recycle
   - Separated by distillation
   - SiI_4 to purification and decomposition
   - I_2 to iodination

6. Operating Ratio
   - Approximately 80% utilization (79.3%)
   - Approximately 7000 hr/year production

7. Recovery of Waste SiI_4
   - Wet recovery of iodine from SiI_4 wastes
   - 90% recovery
   - $ .20/pound of I_2 recovery costs
   - Recycle I_2 to I_2 makeup

8. Storage Considerations
   - Feed materials (two week supply)
   - Product (two week supply)
   - Process (several days)

TABLE 3.1-3

REACTION CHEMISTRY FOR SiI_4 DECOMPOSITION PROCESS

1. Silicon Deposition

$$SiI_4 \rightarrow Si + 2I_2$$

2. Iodination Reaction

$$Si + 2I_2 \rightarrow SiI_4$$

TABLE 3.1-4

RAW MATERIAL REQUIREMENTS FOR SiI_4 DECOMPOSITION PROCESS

Raw Material	Requirement lb/Kg of Silicon
1. Metallurgical Grade Silicon	2.6194
2. Iodine	7.4954

TABLE 3.1-5

UTILITY REQUIREMENTS FOR SiI_4 DECOMPOSITION PROCESS

Utility/Function	K watt-hours/ Kg of Silicon Product*
Heating and Cooling (10% losses)	27.55
Compressor Train	1.059
Radiant Losses from Deposition	190.
	218.61

---

* All utility requirements calculated as electricity. Actual useage would involve cooling water, steam, etc.

TABLE 3.1-6 LIST OF MAJOR PROCESS EQUIPMENT FOR SiI_4 DECOMPOSITION PROCESS

	Item	Function	Duty	Size	Material
1.	Purified SiI_4 Hold Tank	Storage of purified SiI_4 feed to deposition	One Week	6.254×10^4 gallons	316 S.S.
2.	Liquid Storage	Cooled overheads from deposition	One Week	5.6×10^4 gallons	316 S.S.
3.	Silicon Product Storage	Product for sales	Two Weeks	1.097×10^4 gallons	C.S.
4.	Liquid I_2 Storage	I_2 separated from SiI_4	One Week	2.962×10^4 gallons	316 S.S.
5.	SiI_4 Bulk Storage	SiI_4 separated from I_2	One Week	6.948×10^4 gallons	316 S.S.
6.	Metallurgical Silicon Storage	Raw material storage for manufacturing	Two Weeks	1.304×10^4 gallons	C.S.
7.	Feed Tank	Purification column 2 feed tank	Eight Hours	4.008×10^3 gallons	316 S.S.
8.	SiI_4 Vaporizer	Vaporize SiI_4 for deposition unit	+29.86 K cal/gmoles Si produced	121.5 ft^2	C.S. with Hastelloy tubes
9.	Silicon Cooler	Cool product silicon for storage and shipment	-5.7 K cal/gmole Si	ID = 1.85 ft L = 5.67 ft	6 units - Graphit or Quartz
10.	Deposition Condenser	Condense overheads for recycle	-37.146 K cal/gmoles Si	1510.8 ft^2	C.S. with Hastelloy tubes

TABLE 3.1-6 (Continued)

	Item	Function	Duty	Size	Material
11.	Separation Column Preheater	Preheat feed to bubble point for dist.	+3.289 K cal/gmole Si	22.3 ft^2	C.S. with Hastelloy tubes
12.	Separation Column O/H Condenser	Provide liquid reflux to column	−36.66	216.2 ft^2	C.S. with Hastelloy tubes
13.	Separation Column Calandria	Provide vapor rate to column	+42.86	210 ft^2	C.S. with Hastelloy tubes
14.	Separation Column O/H After Cooler	Cool I_2 at B.P. to 130°C for storage	− 2.1	14.24 ft^2	C.S. with Hastelloy tubes
15.	I_2 Vaporizer	Vaporize I_2 for iodination unit	+26.01	113 ft^2	C.S. with Hastelloy tubes
16.	Iodination O/H Condenser	Condense bulk SiI_4 vapors from iodination	−33.85	1377.42 ft^2	C.S. with Hastelloy tubes
17.	Separation Column Bottoms After Cooler	Cool SiI_4 at B.P. to 150°C for storage	− 4.2	28.48 ft^2	C.S. with Hastelloy tubes
18.	Tet Purification Preheater	Bring SiI_4 to bubble point for distillation	+11.41	77.38 ft^2	C.S. with Hastelloy tubes
19.	Purification Column 1 O/H Condenser	Provide reflux for operation of column	−54.42	221 ft^2	C.S. with Hastelloy tubes
20.	Purification Column 1 Calandria	Provide vapor for column operation	54.42	221 ft^2	C.S. with Hastelloy tubes
21.	Purification Column 2 O/H Condenser	Provide reflux for operation of column	−52.24	212 ft^2	C.S. with Hastelloy tubes

TABLE 3.1-6 (Continued)

	Item	Function	Duty	Size	Material
22.	Purification Column 2 Calandria	Provide vapor for operation of column	52.24 K cal/gmole Si	212 ft^2	C.S. with Hastelloy tubes
23.	Purification After Cooler	Cool purified SiI_4 to 150°C for storage	-10.27	69.7 ft^2	C.S. with Hastelloy tubes
24.	De-superheater	Cool for compression	-24.03	163 ft^2 each	6 units - Quartz or Graphite
25.	Purified SiI_4 Pump	Feed to SiI_4 vaporizer	6.2 gpm	100 ft of head	316 S.S.
26.	Deposition Compressor(s)	Return deposition gases to atmospheric pressure	-23.03 K cal/gmole 4.155×10^5 ft^3/min	184.1 horsepower	316 S.S.
27.	I_2/SiI_4 Liquid Pump	Pump to I_2/SiI_4 separation	5.56 gpm	100 ft of head	316 S.S.
28.	I_2/SiI_4 Separation Column Overheads Pump	Pump O/H I_2 for reflux and storage	5.66 gpm	100 ft	316 S.S.
29.	I_2/SiI_4 Separation Column Bottoms Pump	Pump bottoms for reboil and SiI_4 storage	18.45 gpm	150 ft	316 S.S.
30.	I_2 Pump	Pump liquid I_2 through vaporization and iodination	3.[illegible] gpm	150 ft	316 S.S.
31.	SiI_4 Pump	Pump liquid SiI_4 to purification	6.89 gpm	100 ft	316 S.S.
32.	Tet Purification Column 1 O/H Pump	Pump O/H to reflux and waste	19.75 gpm	100 ft	316 S.S.

TABLE 3.1-6 (Continued)

	Item	Function	Duty	Size	Material
33.	Tet Purification Column 1 Bottoms Pump	Pump bottoms for reboil and remove product	27.25 gpm	150 ft	316 S.S.
34.	Tet Purification Column 2 Feed Pump	Feed to Column 2	[illegible].504 gpm	50 ft	316 S.S.
35.	Tet Purification Column 2 O/H Pump	Pump for reflux and to purified stage	18.[illegible] gpm	100 ft	316 S.S.
36.	Tet Purification Column 2 Bottoms Pump	Pump bottoms for reboil and waste	19.35 gpm	150 ft	316 S.S.
37.	Deposition Unit	Produce Si from $SiI_4 \rightarrow Si + 2I_2$	144 Kg of Si/hour + 89.82 K cal/gmole Si	6 at 1018 ft^2 each	Quartz
38.	Iodination Reactor	Produce SiI_4 from met grade Si. $Si + 2I_2 \rightarrow SiI_4$	3263.25 Kg/hr of raw SiI_4, −44.93 K cal/gmoles	23 inch ID by 10 ft tall	Graphite
39.	I_2/SiI_4 Distillation Column	Separate I_2 from SiI_4 for recycle	Separate 1903.36 Kg/hr SiI_4 + 2602.61 Kg/hr I_2	20 ft by 23 inch ID	316 S.S.
40.	Purification Column 1	Purify SiI_4 by 5% cut off top to waste	Feed rate 5166.61 Kg/hr SiI_4	47.6 ft by 26.5 inch ID	316 S.S.
41.	Purification Column 2	Purify SiI_4 by 5% cut off bottom to waste	Feed rate 4908.28 Kg/hr SiI_4	23.8 ft by 26 inch ID	316 S.S.

TABLE 3.1-7 PRODUCTION LABOR REQUIREMENTS OF SiI_4 DECOMPOSITION PROCESS

	Unit Operation	Type	Skilled Man Hrs/Day Unit	Semiskilled Man Hrs/Day Unit
1.	Vaporization	B	23	
2.	Deposition Unit	A	36	
3.	Compression System	B	23	
4.	Vapor Condensation	B	23	
5.	I_2/SiI_4 Distillation	[illegible]	16	
6.	Iodination	B	23	
7.	Tet Purification	C	16	
8.	Materials Handling	A		36
9.	Product Handling	A		36
			160	72

Skilled: .0584 Man-hrs/KgSi

Semiskilled: .0263 Man-hrs/KgSi

TOTAL .0847 Man-hrs/KgSi

NOTES

1. A Batch Process or Multiple Small Units
   B Average Process
   C Automated Process

2. Manhours/Day Unit from Figure 4-6, Peters & Timmerhaus (7).

3.2 Conventional Process for Polysilicon (Siemens Technology)

The chemical engineering analysis activity involves a preliminary process design of a plant to produce polysilicon through the conventional process (Siemens Technology).

The process flowsheet for the conventional polysilicon process, consisting of several major processing operations of hydrochlorination, condensation, distillation and chemical vapor deposition, is shown in Figure 3.2-1.

Initially, metallurgical grade silicon (MGSi) is reacted with anhydrous hydrogen chloride (HCl) in a fluidized bed (550-650°K) to produce a mixture of chlorosilanes, which is primarily trichlorosilane (TCS) and silicon tetrachloride (TET). Since the reactions are highly exothermic, heat transfer for removal of heat of reaction is required to maintain reaction temperature control. The mixture of chlorosilanes from the reaction is condensed and subjected to a several stage distillation to separate by-products and remove impurities.

The purified TCS is reacted with hydrogen (H_2) in a rod reactor to obtain polysilicon deposition via the representative reaction:

$$SiHCl_3 + H_2 \rightarrow Si + 3HCl \qquad (3.2\text{-}1)$$

The deposition reaction occurs on the surface of a hot rod (1000-1100°C) which is heated by passage of electrical current through the rod. Large electrical energy requirements are necessary because of the endothermic reaction, radiation heat losses and incomplete conversion of the TCS. Unreacted chlorosilanes and hydrogen are separated and recycled. Silicon tetrachloride is not recycled.

A process design was performed to obtain data for the cost analysis. The design was based on a plant for the production of 1000 metric tons per year of semiconductor grade polysilicon via the conventional Siemens process.

The detailed status sheet for the process design package is shown in Table 3.2-1 and is representative of the various sub-items that make up the activity. 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:

- Base Case Conditions--------------Table 3.2-2
- Reaction chemistry----------------Table 3.2-3
- Raw Material Requirements---------Table 3.2-4
- Utility Requirements--------------Table 3.2-5
- Major Process Equipment-----------Table 3.2-6
- Production Labor Requirements----Table 3.2-7

The process design provides detailed data for raw materials, utilities, major process equpment and production labor requirements which are necessary for polysilicon production.

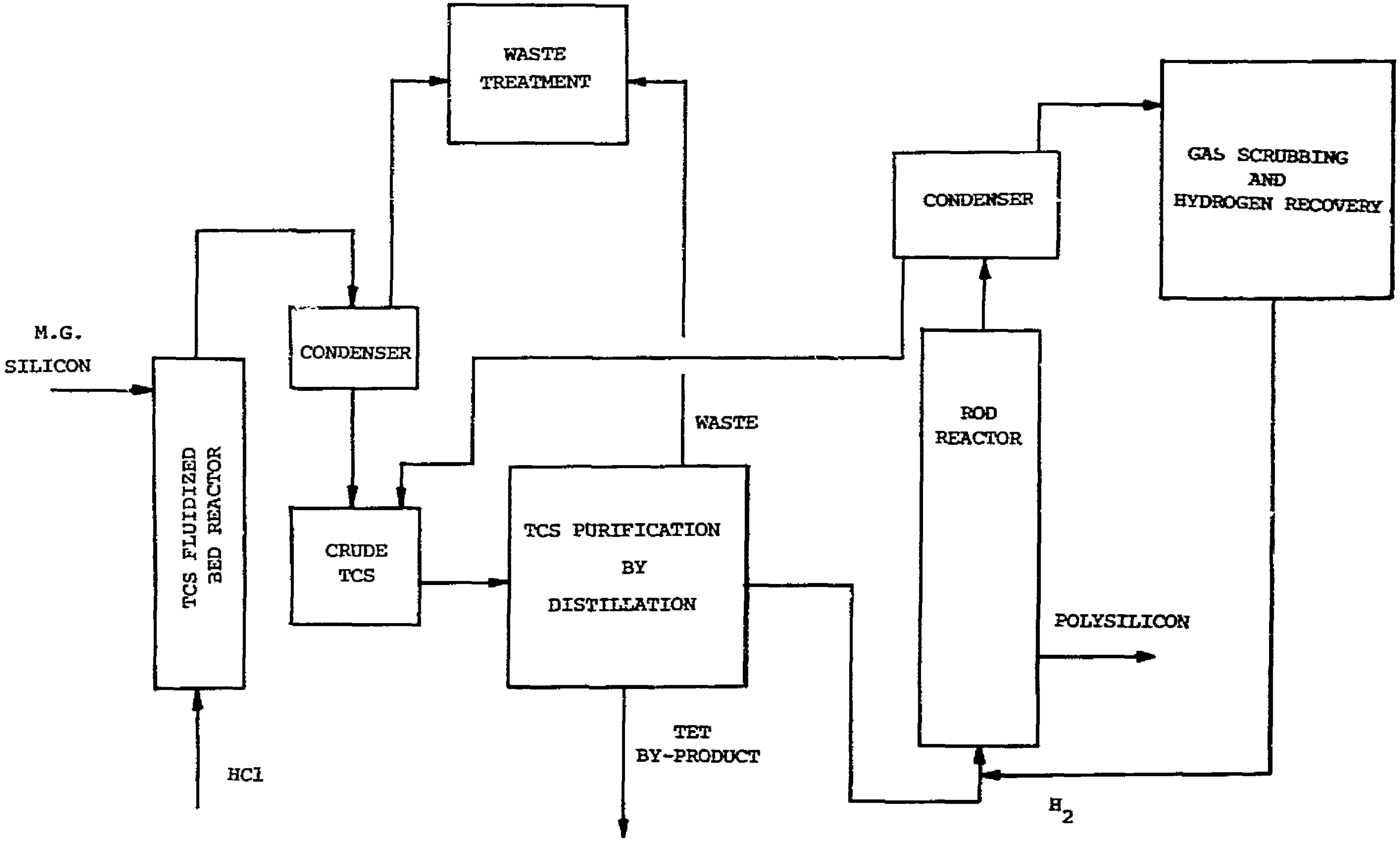

Figure 3.2-1 Preliminary Process Flowsheet for Conventional Polysilicon Process

TABLE 3.2-1 CHEMICAL ENGINEERING ANALYSES:
PRELIMINARY PROCESS DESIGN ACTIVITIES FOR CONVENTIONAL POLYSILICON PROCESS

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

○ Plan
◐ In Progress
● Complete

TABLE 3.2-2
BASE CASE CONDITIONS FOR CONVENTIONAL POLYSILICON PROCESS

1. Plant Size
   - 1000 metric tons per year
   - Semiconductor grade silicon

2. Production of TCS
   - Fluidized Bed, 600°K, low pressure (65 PSIA)
   - Metallurgical grade silicon plus HCl gas
   - Chlorosilane content in condensed reator gas by moles (ref. 32)

     91.5% TCS ($SiCl_3H$)
     5.2% TET ($SiCl_4$)
     1.4% DCS ($SiCl_2H_2$)
     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_2

   - 8.17 moles TCS in/mole of Si production in an <u>operating</u> reactor
   - Exit gas analysis (ref. 20)

     4.339% TET
     4.457% TCS
     .089% DCS
     2.197% HCl
     88.92% H_2

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 3.2-2 (Continued)

6. Recycles
   - H_2 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

TABLE 3.2-3

REACTION CHEMISTRY FOR CONVENTIONAL POLYSILICON PROCESS

1. TCS Reactor

$Si + 3\ HCl \rightarrow SiHCl_3 + H_2$

$Si + 4\ HCl \rightarrow SiCl_4 + 2H_2$

$Si + 2HCl \rightarrow SiH_2Cl_2$

2. Rod Reactor

$SiHCl_3 + H_2 \rightarrow Si + 3HCl$

$SiHCl_3 + HCl \rightarrow SiCl_4 + H_2$

$SiHCl_3 + H_2 \rightarrow SiH_2Cl_2 + HCl$

3. Waste Treatment

$SiHCl_3 + 2H_2O \rightarrow SiO_2 + 3HCl + H_2$

$SiCl_4 + 2H_2O \rightarrow SiO_2 + 4HCl$

$SiH_2Cl_2 + 2H_2O \rightarrow SiO_2 + 2HCl + 2H_2$

$HCl + NaOH \rightarrow NaCl + H_2O$

TABLE 3.2-4

RAW MATERIAL REQUIREMENTS FOR CONVENTIONAL POLYSILICON PROCESS

	Raw Material	Requirement lb/Kg of Silicon
1.	M. G. Silicon	6.72 Kg/Kg
2.	Anhydrous HCl	57.96
3.	Hydrogen	.828
4.	Caustic (50% NaOH)	53.29
5.	$SiCl_4$ (By Product)	46.12

TABLE 3.2-5

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. Steam (250 PSIA)		152 Pounds
1. HCl Vaporizer	(7.07)	
2. Caustic Storage Tank	(1.82)	
3. #1 Scrubber Vapor Heater	(.276)	
4. #1 Distillation Column Calandria	(38.75)	
5. #2 Distillation Column Calandria	(47.73)	
6. #3 Distillation Column Calandria	(25.24)	
7. TCS Vaporizer	(10.79)	
8. #2 Scrubber Vapor Heater	(3.4)	
9. Liquid Recycle Heater	(5.52)	
10. #4 Distillation Column Calandria	(11.3)	
11. Rod Reactor	(-1287 generated)	
3. Cooling Water		984.5 Gallons
1. TCS Reactor Off Gas Cooler	(13.91)	
2. Rod Reactor Off Gas Cooler	(334)	
3. #4 Distillation Column Condenser	(37.24)	
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°F)		42.1 M BTU
1. TCS Reactor Off Gas Condenser	(12.57)	
2. Rod Reactor Off Gas Condenser	(29.52)	
6. Refrigerant (34°F)		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. High Temperature Heat Exchange Fluid		582 Pounds
1. TCS Fluidized Bed Reactor	(581)	
2. Nitrogen Heater	(0.61)	
8. Nitrogen		349.1 SCF
1. Molecular Sieves	(328.5)	
2. Polysilicon Rod Reactor Purge	(20.64)	

TABLE 3.2-6

LIST OF MAJOR PROCESS EQUIPMENT FOR CONVENTIONAL POLYSILICON PROCESS

		Type	Function	Duty	Size	Materials of Construction
1.	(T1)	M.G. Silicon Storage Hopper	Raw Material Storage	2 Weeks Storage	6.5×10^4 gallons	CS
2.	(T2)	Liquid HCl Storage Tank	Raw Material Storage	2 Weeks Storage	2.5×10^5 gallons 250 PSIA	Nickel Steel
3.	(T3)	Crude TCS Hold Tanks (3)	Feed for Purification	1 Week Storage	2.77×10^5 gallons (each)	CS
4.	(T4)	Waste Hold Tank	Feed For Waste Treatment	1 Week Storage	3.025×10^4 gallons	CS
5.	(T5)	TCS Reactor Off Gas Flash Tank	Phase Separation		1 ft. in diameter by 4 ft. tall, 300 PSIA	SS
6.	(T6)	Hydrogen Storage Tank	Make-up For Losses	8 Hours Backup for Pipeline Failure	7.24×10^4 gallons Spherical 250 PSIA	CS
7.	(T7)	Polysilicon Storage Space	Final Product Storage	2 Weeks Storage	1300 ft.^3 of space	CS
8.	(T8)	TET Storage Tanks (2)	Final By-product Storage	2 Weeks Storage	1.62×10^5 Gallons (each)	CS
9.	(T9)	TET Feed Tanks (2)	Feed for Distillation Column #4	1 Week Storage	8.83×10^4 Gallons (each)	CS
10.	(T10)	TCS Feed Tanks (3)	Feed for Distillation Column #3	1 Day Storage	2.47×10^4 Gallons (each)	CS
11.	(T11)	TCS Storage Tanks (3)	Purified TCS Hold-Up Feed to Rod Reactor	1 Week Storage	1.64×10^5 Gallons (each)	CS
12.	(T12)	TET/TCS Feed Tanks (3)	Feed for Distillation Column #2	1 Day Storage	3.75×10^4 Gallons (each)	CS

TABLE 3.2-6 (continued)

13.	(T13)	Caustic Storage Tank	Raw Material Storage	2 Week Storage 1.91×10^5 BTU/HR	1.82×10^5 Gallons	SS
14.	(T14)	#1 Distillation Condenser Flash Tank	Phase Separation		1 Ft. in Diameter by 4 Feet Tall	CS
15.	(T15)	Rod Reactor Off Gas Flash Tank	Phase Separation		1 Ft. in Diameter by 4 Feet Tall 300 PSIA	SS
16.	(H1)	HCl Vaporizer	Vaporize Feed To TCS Reactor	7.5×10^5 BTU/Hr	38.29 Ft.^2 250 PSIA Shell	SS/SS
17.	(H2)	TCS Reactor Off Gas Cooler	Cool Reaction Gas	4.4×10^5 BTU/Hr	224 Ft.^2 65 PSIA Tubes	CS/SS
18.	(H3)	TCS Reactor Off Gas Condenser	Condense Reaction Gas	1.6×10^6 BTU/Hr	1423 Ft.^2 300 PSIA Tubes	SS/SS
19.	(H4)	#1 Scrubber Vapor Heater	Heat Vapor Wastes to 40°F for Scrubbing	3×10^4 BTU/Hr	15.7 Ft.^2 250 PSIA Shell	CS/SS
20.	(H5)	#1 Distillation Column Condenser	Condense Overheads for Relux	4.31×10^6 BTU/Hr	1540 Ft.^2	CS/SS
21.	(H6)	#1 Distillation Column Calandria	Reboiler for Column #1	4×10^6 BTU/Hr	311. Ft.^2 250 PSIA Shell	CS/SS
22.	(H7)	#2 Distillation Column Condenser	Condense Overheads For Reflux	4.7×10^6 BTU/Hr	1555 Ft.^2	CS/CS
23.	(H8)	#2 Distillation Column Calandria	Reboiler for Column #2	5×10^6 BTU/Hr	402.4 Ft.^2 250 PSIA Shell	CS/SS
24.	(H9)	#3 Distillation Column Condenser	Condense Overheads for Reflux	2.64×10^6 BTU/Hr	867 Ft.^2	CS/CS

TABLE 3.2-6 (continued)

25.	(H10)	#3 Distillation Column Calandria	Reboiler for Column #3	2.64×10^6 BTU/Hr	173 Ft.^{2} 250 PSIA Shell	CS/SS
26.	(H11)	TCS Vaporizer	Vaporize Feed To Rod Reactor	1.13×10^6 BTU/Hr	3 Ft.^{2} 250 PSIA Shell	CS/CS
27.	(H12)	Rod Reactor Off Gas Cooler	Cool Reaction Gas	1.06×10^7 BTU/Hr	2519 Ft.^{2} 20 PSIA	CS/SS
28.	(H13)	Rod Reactor Off Gas Condenser	Condense Reaction Gas	3.74×10^6 BTU/Hr	3341 Ft.^{2} 300 PSIA Tubes	SS/SS
29.	(H14)	#2 Scrubber Vapor Heater	Heat Vapor Wastes to 40°F for Scrubbing	3.56×10^5 BTU/Hr	180 Ft.^{2} 250 PSIA Shell	CS/SS
30.	(H15)	Liquid Recycle Heater	Heat Cold Recycle Liquid (Crude TCS) to 80°F for Storage	5.79×10^5 BTU/Hr	30.6 Ft.^{2} 250 PSIA Shell	SS/SS
31.	(H16)	#4 Distillation Column Condenser	Condenser Overheads for Reflux	1.18×10^6 BTU/Hr	513 Ft.^{2}	CS/CS
32.	(H17)	#4 Distillation Column Calandria	Reboiler for Column #4	1.18×10^6 BTU/Hr	95 Ft.^{2} 250 PSIA Shell	CS/SS
33.	(H18)	Nitrogen Heater	Heat Regenerator Gas for Molecular Sieves	2.46×10^4 BTU/Hr	44.8 Ft.^{2}	CS/CS
34.	(P1)	TCS Reactor Off Gas Compressor	Compress Reaction Gas For Condensation	3.52×10^5 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)	#1 Distillation Column Overheads Pump	Supply Reflux and Remove Waste to Waste Hold Tank		62.2 gpm 100 Ft. of Head	CS*

TABLE 3.2-6 (continued)

37.	(P4)	#1 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*
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	3.65×10^6 BTU/Hr	1434 Horsepower	CS
46.	(P13)	#4 Distillation Column Overheads Pump	Supply Reflux Pump TET by product to TET Storage Tank		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

*Includes incremental higher cost for special purity requirements.

TABLE 3.2-6 (continued)

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)	#1 Gas Scrubber	Scrub Gas Wastes from TCS Reactor Off Gas		43 Ft. Tall D = 3½ Ft.	SS
53.	(C2)	#2 Gas Scrubber	Scrub Gas Wastes from H16, H3, H5		40 Ft. Tall D = 2¼ Ft.	SS
54.	(C3)	#1 Distillation Column	Separate Light Impurities to Waste		29 Trays 24 inches apart 3 3/4 Ft. in Diameter	CS
55.	(C4)	#2 Distillation Column	Separate TET and TCS		29 Trays 24 inches apart 4¼ 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.	(R1)	TCS Fluidized Bed Reactor	Production of TCS For Rod Reactor	4.552×10^6 BTU/Hr (Cooling)	D = 2.61 Ft. L = 28.8 Ft. 64, 1" O D Cooling Tubes 9.4' Long	SS

TABLE 3.2-6 (continued)

59.	(R2)	Polysilicon Rod Reactors (305)	Production of Polysilicon		Hairpin Reactor (2 hairpins, 3 Ft. long, 6 Inch Dia.)	Quartz
60.	(A1)	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	8.94×10^6 BTU/Hr	30 Feet High Stack 6" diameter	CS
63.	(A4)	Filament Pullers	Production of 1/4" filaments for Polysilicon depositon			

TABLE 3.2-7

PRODUCTION LABOR REQUIREMENTS FOR CONVENTIONAL POLYSILICON PROCESS

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

NOTES:

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.

3.3 UCC Silane Process for Silicon (Union Carbide Corporation)

The chemical engineering analysis activity involves a preliminary process design of a plant to produce silicon via the technology under consideration.

The UCC silane process (Union Carbide Corporation) for silicon involves several processing operations of hydrogenation-hydrochlorination reaction, stripping, distillation, redistribution reaction, silane purification, pryolysis and consolidation of silicon. The process flowsheet is shown in Figure 3.3-1.

Hydrogen, silicon tetrachloride, and metallurigical grade silicon are fed to the hydrogenation reactor (fluidized bed, 500°C, 515 psia, copper catalyst) to produce a mixture of chlorosilanes. The mixture of chlorosilanes from the hydrogenation reaction is condensed and subjected to several state distillation to separate components and remove impurities.

Initially, the condensed liquid mixture is sent to D-01 stripper (90 psia) to remove inert gases and volatile impurities. The stripper bottoms go to D-02 distillation (55 psia) which separates TCS (trichlorosilane) and STC (silicon tetrachloride). The TCS redistribution reactor (liquid phase, 85 psia, 140°F catalyst) is used to produce DCS (dichlorosilane). The separation of DCS and TCS is achieved in D-03 distillation (320 psia). The overhead goes to DCS redistribution reactor (liquid phase, 510 psia, 140°F, catalyst) to produce silane (SiH_4). The silane is purified by separation from trace impurities (such as B_2H_6) by D-04 distillation (355 psia).

The purified silane is used to produce silicon powder via the pyrolysis reaction:

$$SiH_4 \rightarrow Si + 2H_2. \qquad (3.3\text{-}1)$$

The hydrogen from the reaction is compressed and recycled to the hydrogenation reactor. The silicon powder from the pyrolysis is consolidated to provide the molten silicon product.

A process design was performed to obtain data for a cost analysis of a plant to produce silicon by this new technology. The design was based on a plant to produce 1000 metric tons/yr of silicon via the UCC silane process.

The detailed status sheet for the process design package is shown in Table 3.3-1, and is representative of the various sub-items that make up the activity. 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:

- Process Flowsheet------------------Figure 3.3-2
- Base Case Conditions---------------Table 3.3-2
- Reaction Chemistry-----------------Table 3.3-3
- Redistribution Equilibrium---------Figure 3.3-3
- Raw Material Requirements----------Table 3.3-4
- Utility Requirements---------------Table 3.3-5
- Major Process Equipment------------Table 3.3-6
- Production Labor Requirements------Table 3.3-7

The process design provides detailed data for raw materials, utilities, major process equipment and production labor requirements which are necessary for polysilicon production.

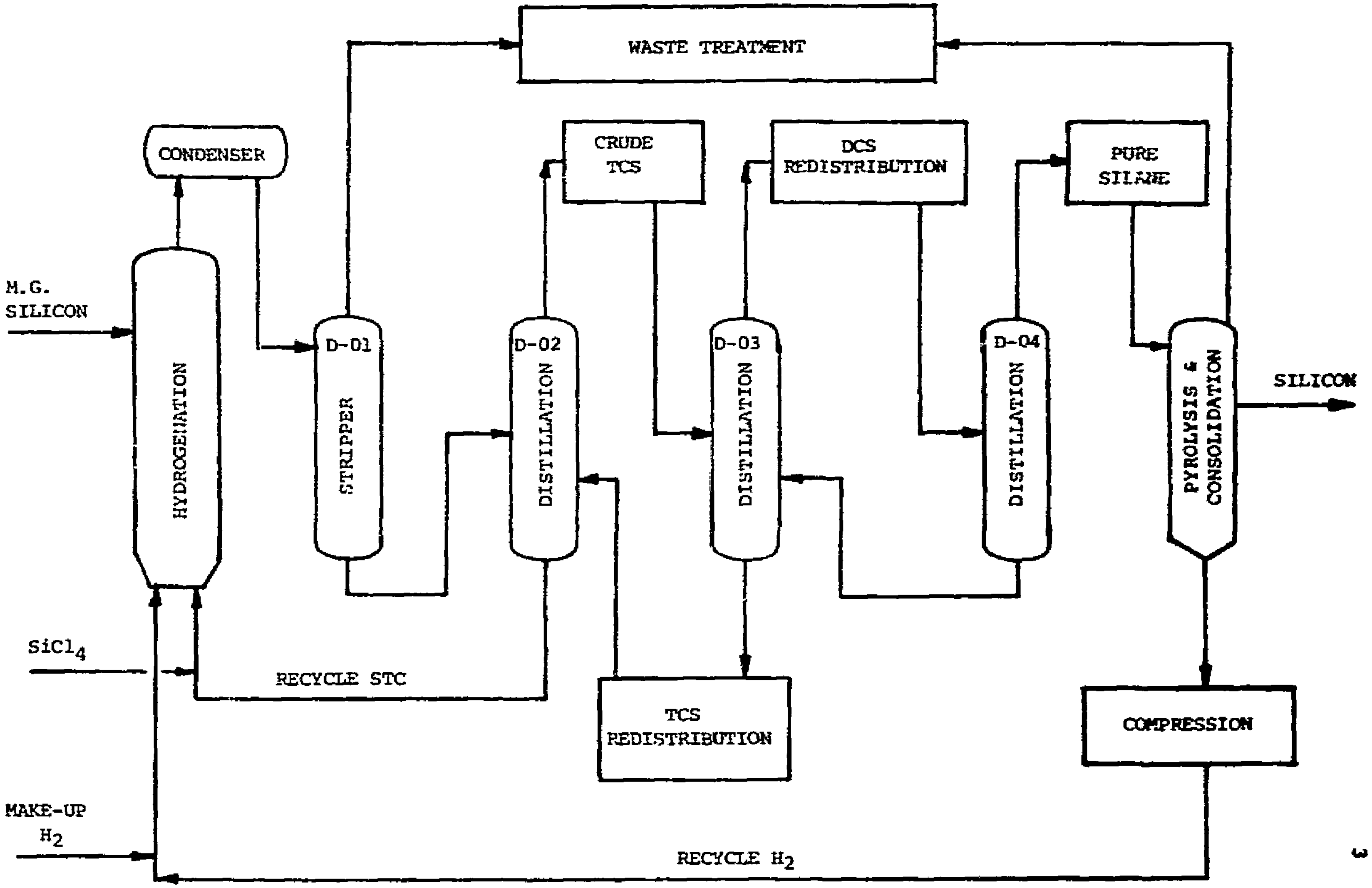

Figure 3.3-1 PROCESS FLOWSHEET FOR UCC SILANE PROCESS

TABLE 3.3-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR UCC SILANE PROCESS

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

○ Plan
◐ In Progress
● Complete

CASE C

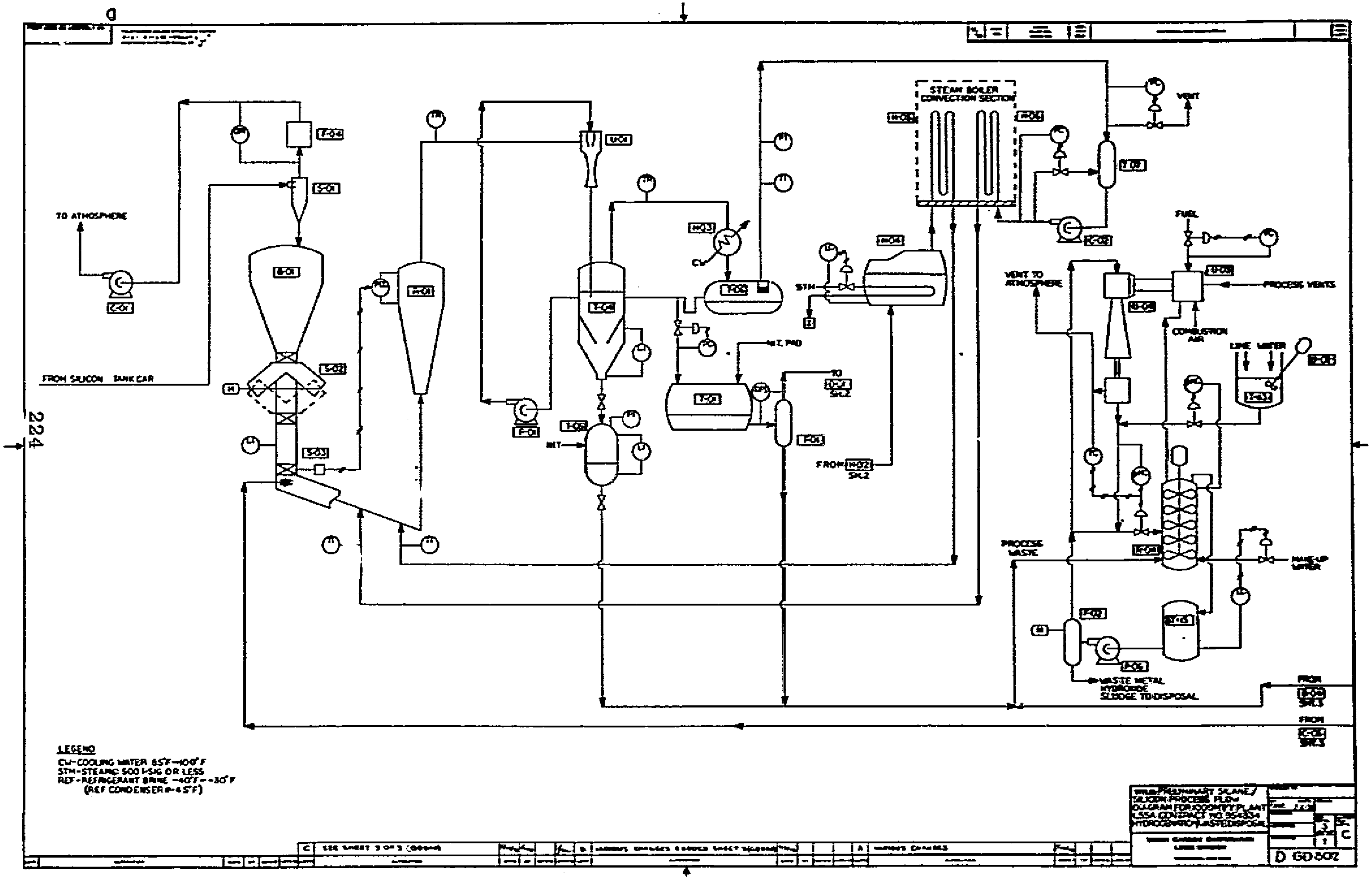

Figure 3.3-2 Process Flow Sheet for UCC Silane Process

CASE C

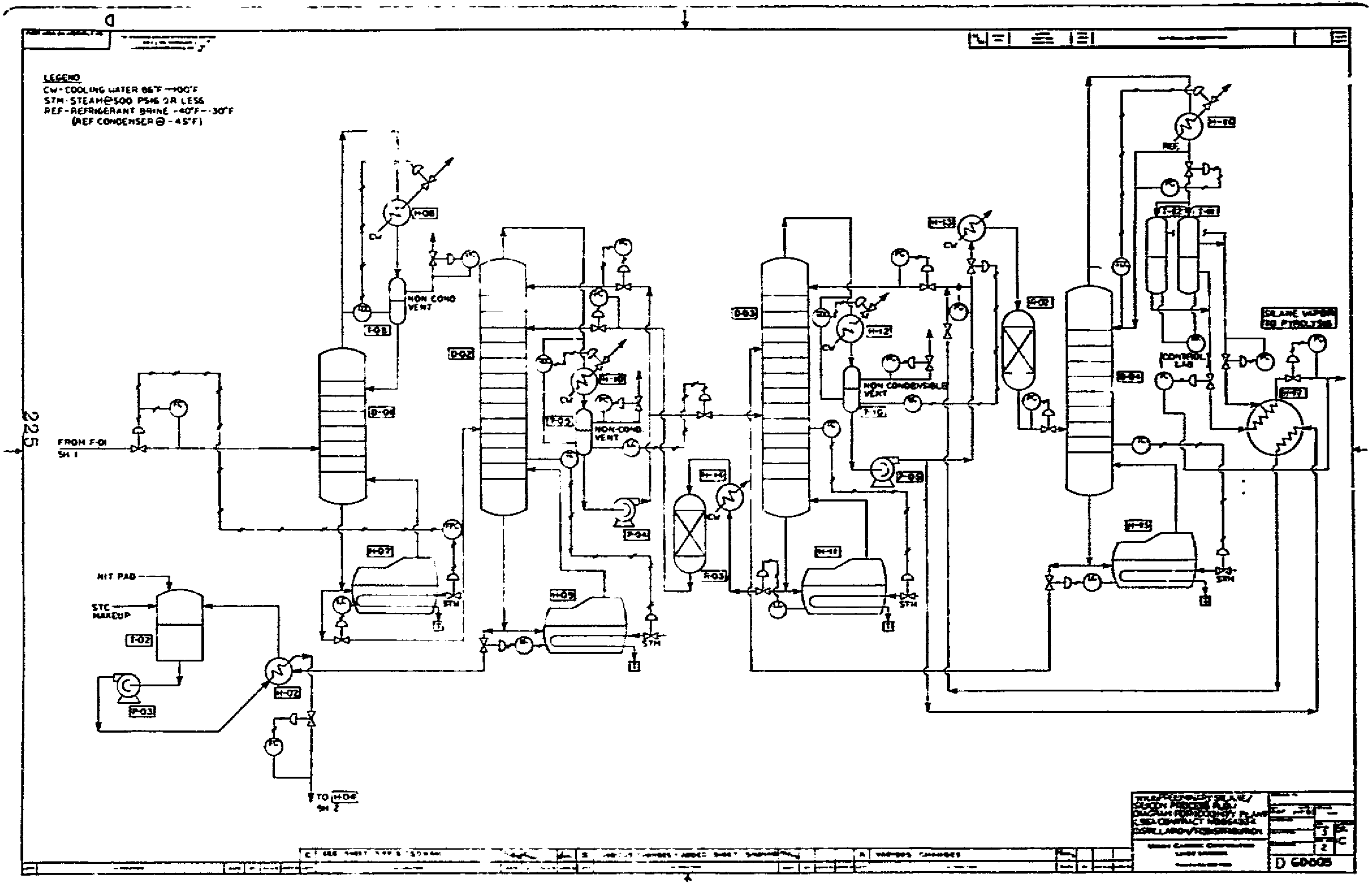

Figure 3.3-2 (Continued)

CASE C

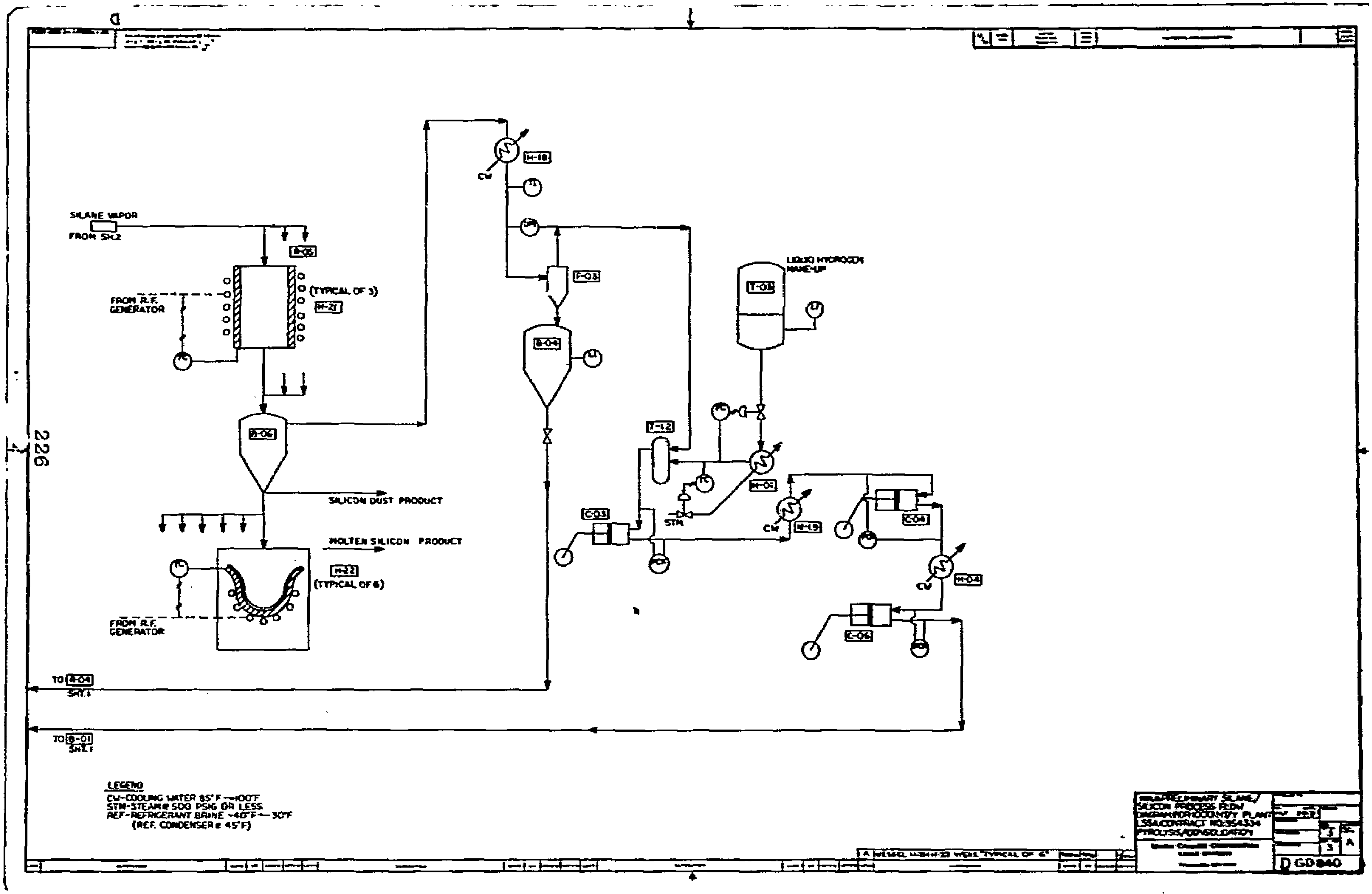

Figure 3.3-2 (Continued)

CASE C

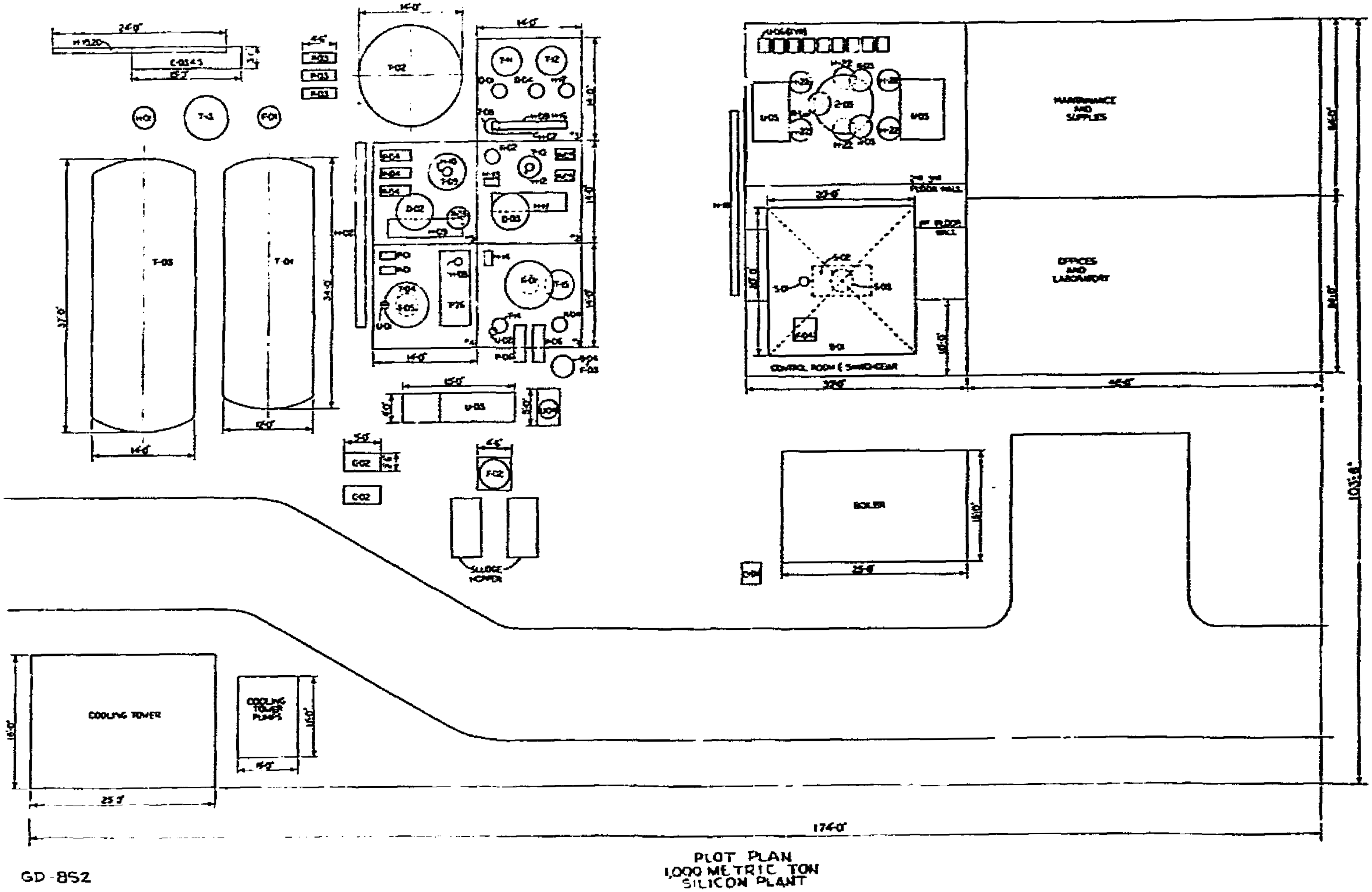

Figure 3.3-2 (Continued)

TABLE 3.3-2

BASE CASE CONDITIONS FOR UCC SILANE PROCESS

1. Plant Size
   - Silicon produced from silane
   - 1000 metric tons/year of silicon
   - Solar cell grade silicon
2. Hydrogenation Reaction
   - Metallurgical grade silicon, hydrogen, and recycle silicon tetrachloride (TET) used to produce trichlorosilane (TCS)
   - Copper catalyzed
   - Fluidized bed
   - 500°C, 514.7 psia
   - 20% to 22.5% conversion of $SiCl_4$ (example)
3. TCS Redistribution Reaction
   - TCS from hydrogenation produces dichlorosilane (DCS)
   - Catalytic redistribution of TCS with tertiary amine ion exchange resin
   - Liquid phase 85 psia, 140°F
   - Conversion a function of inlet concentration (Union Carbide equilibrium)
   - Conversion from pure TCS feed is about 9.5% to DCS (example)
4. DCS Redistribution Reaction
   - DCS produces SiH_4 (silane)
   - Catalytic redistribution of DCS with tertiary amine exchange resin
   - Liquid phase 510 psia, 140°F
   - Conversion a function of inlet concentration (Union Carbide equilibrium)
   - Conversion from pure DCS feed is about 14% to Silane (example)
5. Recycles
   - Unreacted chlorosilanes separated by distillation and recycled
6. Silane Purification
   - Final purification by distillation
   - Designed to remove trace impurities (B_2H_6, example)
7. Operating Ratio
   - Approximately 85% utilization (on stream time)
   - Approximately 7445 hour/year production
8. Storage Consideration
   - Feed materials (several week supply, approx. 1 month)
   - Product (two shifts storage)
   - Process (several hours to 1 shift)

TABLE 3.3-3

REACTION CHEMISTRY FOR UCC SILANE PROCESS

1. Hydrogenation Reaction

$$3\ SiCl_4 + Si + 2H_2 \rightleftarrows 4\ SiHCl_3$$

2. Trichlorosilane Redistribution Reaction

$$2\ SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4$$

3. Dichlorosilane Redistribution Reaction

$$3\ SiH_2Cl_2 \xrightarrow{\text{Distillation}} 2\ SiHCl_3 + SiH_4$$

4. Waste Treatment (representative)

$$SiH_2Cl_2 + Ca(OH)_2 \xrightarrow{aq.} SiO_2 + CaCl_2 + 2H_2O$$

$$SiHCl_3 + 1.5Ca(OH)_2 \xrightarrow{aq.} SiO_2 + 1.5CaCl_2 + 2H_2O$$

$$SiCl_4 + 2Ca(OH)_2 \xrightarrow{aq.} SiO_2 + 2CaCl_2 + 2H_2O$$

5. Silane Pyrolysis Reaction

$$SiH_4 \longrightarrow Si + 2H_2$$

Note

1. Reaction 1 product contains H_2, HCl, $SiCl_4$, $SiHCl_3$, SiH_2Cl_2(trace), other trace chlorides
2. Reaction 2 Product contains $SiHCl_3$ $SiCl_4$, SiH_2Cl_2, SiH_3Cl
3. Reaction 3 Product contains SiH_2Cl_2, $SiHCl_3$, $SiCl_4$, SiH_3Cl, SiH_4

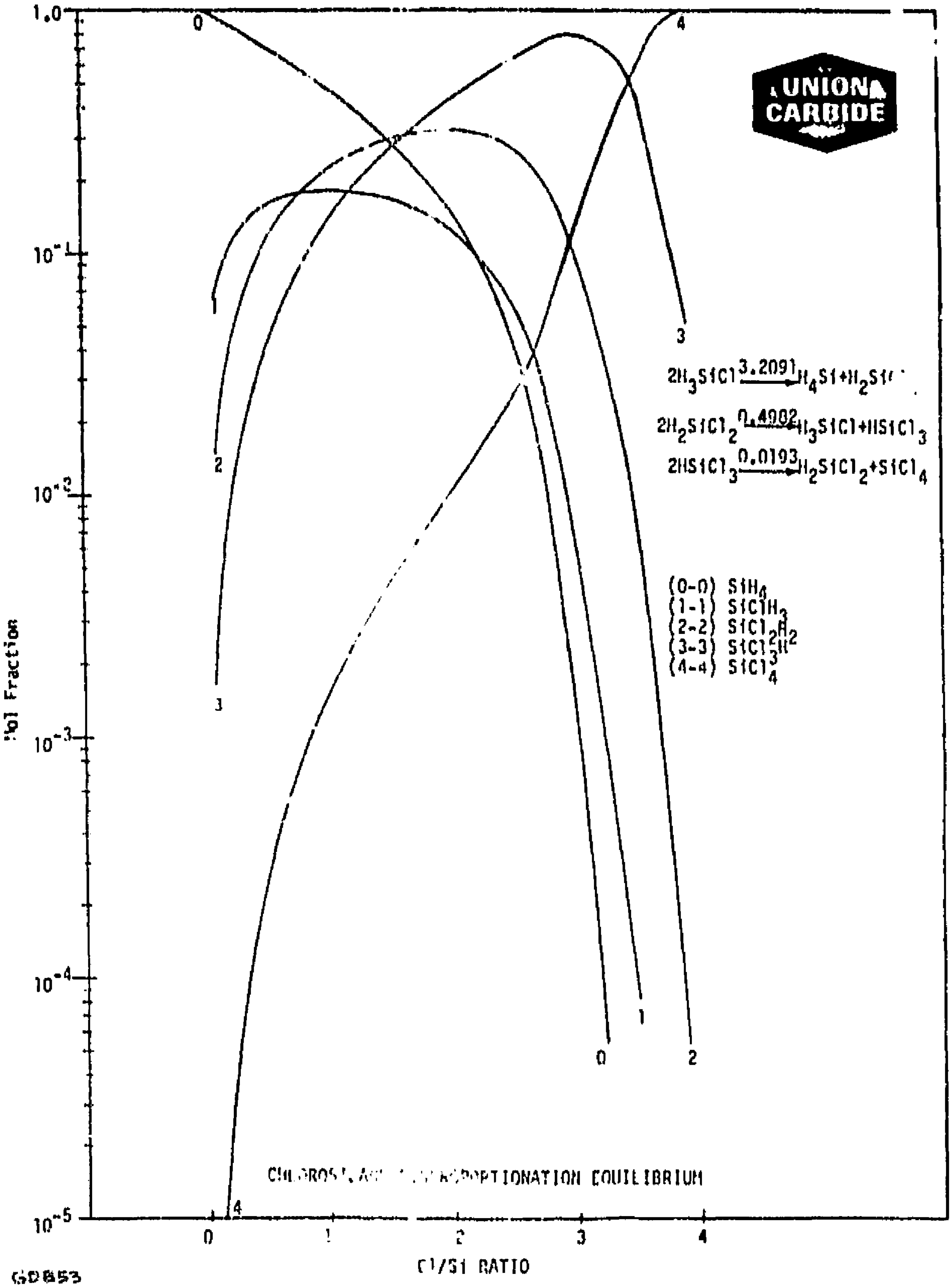

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Figure 3.3-3 Redistribution Equilibrium For UCC Silane Process (Provided by Union Carbide)

TABLE 3.3-4

RAW MATERIAL REQUIREMENTS FOR UCC SILANE PROCESS

	Raw Material	Requirements	
		lb/hr for 1000 MT/yr Silicon	lb/KG of Silicon
1.	M. G. Silicon (Si)	348.6	2.60
2.	Silicon Tetrachloride ($SiCl_4$, make-up)	370.1	2.76
3.	Liquid Hydrogen (H_2, make-up)	4.3	0.032
4.	Copper Catalyst (Cu)	6.8	0.051
5.	Hydrate Lime [$Ca(OH)_2$]	326.3	2.43

Note:

Assuming all inert gas from D-01 is H_2

TABLE 3.3-5

UTILITY REQUIREMENTS FOR UCC SILANE PROCESS

Utility/Function	Total Requirement	Requirement/KG Silicon
1. Electricity	409.7 KW	3.050 KW/hr
2. Steam	23113 lb/hr	172.2 lbs.
3. Cooling Water	70,453 gal/hr	525 gallons
4. Process Water	9.52 gal/hr	0.0709 gallons
5. Refrigerant	0.130 MM Btu/hr	968 Btu
6. Fuel	3.640 MM Btu/hr	27,100 Btu

TABLE 3.3-6

LIST OF MAJOR PROCESS
EQUIPMENT FOR UCC SILANE PROCESS

	Equipment	Function	Duty/Type	Size	Material of Construction
DISTILLATION COLUMNS					
1.	D-01 Crude TCS/STC Stripping Column	To remove inert gases	24929 lb/hr of feed	24" diam. 20' tall, 10 sieve plates	CS
2.	D-02 TCS/STC Distillation Column	To remove STC at bottoms	64,213 lb/hr of feeds	4.63' diam., 74' tall, 32 sieve plates	CS
3.	D-03 DCS/TCS Distillation Column	To remove DCS at distillates	46,254 lb/hr of feeds	4.30' diam., 77.5' tall, 45 sieve plates	CS
4.	D-04 Silane Distillation Column	To purify silane	6967 lb/hr of feed	24" diam., 50'tall, 30 sieve plates	316SS
REACTORS					
5.	R-01 Hydrogenation Reactor (Fluidized Bed)	Hydrogenation of Si and $SiCl_4$	25,447 lb/hr of feed	6.5' diam. x 6.5'/ 2.5' diam. x 10.5' cone	316SS
6.	R-02 DCS Redistribution Reactor (Fixed Bed)	To convert DCS to silane	6,967 lb/hr of feed	2' diam., 11.2' tall, with catalyst	316SS
7.	R-03 TCS Redistribution Teactor (Fixed Bed)	To convert TCS to DCS and STC	39,287 lb/hr of feed	3' diam., 17.3' tall, with catalyst	316SS
8. & 9.	R-04 Sludge Neutralization Reactor	Waste Treatment	Agitated Tank/Column	2' diam., 20' tall	316SS (for pricing)

TABLE 3.3-6 (Continued)

HEAT EXCHANGERS

10.	H-01 Liquid Hydrogen Vaporizer	To provide H_2 gas	7.22 lb/hr of Liquid H_2	(Vendor supplied equipment)	
11.	H-02 STC Cooler	Exchange heats of STC streams	7.23×10^5 Btu/hr shell-tube H. E.	893 ft.^{2} 514.7 psia	316SS/CS
12.	H-03 Quench Condenser	To condense chlorosilanes, 100°F	4.69×10^6 Btu/hr shell-tube H. E.	676 ft.^{2} 514.7 psia	316SS/CS
13.	H-04 Recycle STC Vaporizer	To provide STC vapor to reactor	1.71×10^6 Btu/hr kettle	65.9 ft.^{2} 514.7 psia	CS
14.	H-05 Recycle STC Superheater	To heat STC from 234 to 932°F	2.46×10^6 Btu/hr Furnace Convection	1603 ft.^{2} 514.7 psia	316SS
15.	H-06 Recycle H_2 Heater	To heat H_2 from 100 to 932°F	6.78×10^5 Btu/hr Furnace Convection	331 ft.^{2} 514.7 psia	316SS
16.	H-07 Stipper Recoiler	Reboiler of D-01, 242°F	9.06×10^5 Btu/hr Kettle	39.8 ft.^{2} 95 psia	CS
17.	H-08 Stripper Condenser	Partial Condenser of D-01, 139°F	86,700 Btu/hr shell-tube H. E.	36.1 ft.^{2} 90 psia	CS
18.	H-09 TCS/STC Reboiler	Reboiler of D-02 216°F	7.83×10^6 Btu/hr kettle	295 ft.^{2} 55 psia	CS
19.	H-10 TCS/STC Condenser	Total condenser of D-02, 120°F	6.24 x 10[illegible] Btu/hr shell-tube H. E.	1315 ft.^{2} 55 psia	316SS/CS

TABLE 3.3-6 (Continued)

20.	H-11 DCS/TCS Reboiler	Reboiler of D-03	3.50×10^6 Btu/hr Kettle	333 $ft.^2$ 320 psia	CS
21.	H-12 DCS/TCS Condenser	Total condenser of D-03, 234°F	3.99×10^6 Btu/hr shell-tube H. E.	429 $ft.^2$ 320 psia	316SS/CS
22.	H-13 DCS Cooler	To cool DCS before redistribution reaction	1.88×10^5 Btu/hr shell-tube H. E.	22.1 $ft.^2$ 550 psia	316SS/CS
23.	H-14 TCS Cooler	To cool TCS before redistribution reaction	2.01×10^6 Btu/hr shell-tube H. E.	161 $ft.^2$ 85 psia	316SS/CS
24.	H-15 Silane Boiler	Reboiler of D-04 278°F	2.71×10^5 Btu/hr Kettle	15.4 $ft.^2$ 360 psia	316SS/CS
25.	H-16 Silane Condenser	Total conderser of -44PF	1.30×10^5 Btu/hr Shell-tube H. E.	81 $ft.^2$ 360 psia	316SS
26.	H-17 Silane Vaporizer/Superheater	To provide silane vapor for pyrolysis, 200°F	25,000 Btu/hr Jacket/tubes	27.3 $ft.^3$/12.0 $ft.^2$ 355 psia	316SS/CS
27.	H-18 Pyrolysis Hydrogen Cooler	To cool H_2 gas from 363 to 100°F	43,000 Btu/hr shell-tube H. E.	80.5 $ft.^2$ 20 psia	316SS/CS
28.	H-19 First Stage H_2 Intercooler	To cool H_2 between comp. stages 328 to 100°F	38,570 Btu/hr shell-tube H.E.	72.2 $ft.^2$ 50 psia	316SS/CS
29.	H-20 Second Stage H_2 Intercooler	To cool H_2 between comp. stages 328 to 100°F	38570 Btu/hr shell-tube H. E.	72.2 $ft.^2$ 160 psia	316SS/CS

TABLE 3.3-6 (Continued)

PUMPS AND COMPRESSORS

30.	C-01 Pneumatic Conveying Fan	Si feed transport	417 ACFM Centrifugal	5.1 psi Δp 12 BHP	CS
31.	C-02 Recycle H_2 Blower	H_2 gas blower	22.8 ACFM Centrifugal	518.7 psia 1.23 BHP	CS
32.	C-03 First Stage H_2 Compressor	H_2 gas compressor	164 ACFM; double action, reciprocating	48.1 psia discharge, 19.8 BHP	CS
33.	C-04 Second Stage H_2 Compressor	H_2 gas compressor action,	50 ACFM; double action, reciprocating	157 psia discharge, 19.6 BHP	CS
34.	C-05 Third Stage H_2 Compressor	H_2 gas compressor	15.3 ACFM;double action, reciprocating	515 psia discharge, 19.8 BHP	CS
35.	P-01 Quench Contactor Pump	Circulating liquid chlorosilanes	100 gpm, centrifugal/motor	36.7' head, 1.56 BHP	316SS
36.	P-03 Recycle STC Pump	To supply STC	33.1 gpm Centrifugal/ Turbine	847' head, 14.2 BHP	CS
37.	P-04 TCS Distillate Pump	D-02 Reflux/ Distillate	144 gpm Centrifugal/ Turbine	589' head, 33.5 BHP	CS
38.	P-05 DCS Distillate Pump	D-03 Reflux/ Distillate	144 gpm Centrifugal/ Motor	759' head, 26.2 BHP	316SS
39.	P-06 Lime Tank Pump	Circulating Lime Slurry	100 gpm Centrifugal/ Motor	103' head, 4.BHP	Cast iron

TABLE 3.3-6 (Continued)

TANKS AND BINS

40.	T-01 Crude TCS/STC Storage Tank	Storage/Feed to Silane production	8 hr. storage, horizontal	12' diam. x 27' [illegible] psia	CS
41.	T-02 STC Storage Tank	Storage/Feed to Hydrogenation	6 hr. storage, Vertical	14' diam. x 13.4' 14.7 psia	CS
42.	T-03 Liq. H_2 Storage	Liq. H_2 make-up storage	(Vendor supplied equipment)		
43.	T-04 Waste Settler Tank	To separate solid residues	Vertical cyl/cone bottom	6' diam., 12' tall 514.7 psia	316SS
44.	T-05 Waste Chlorides Tank	To remove solid residues	285 lb/hr Vertical	3' diam., 4' tall 25 psia (aprox.)	316SS
45.	T-06 Quench Condenser Receiver	Gas-liq. separa-	15 min. storage Horizontal	4' diam. x 11.3' 514.7 psia	CS
46.	T-07 Recycle Hydrogen Receiver	H_2 gas surge tank	Vertical	3' diam. x 6' 514.7 psia	CS
47.	T-08 Stripper Reflux pot	D-01 Distillate/ gas	30 min. storage Vertical	2' diam. x 3.4' 90 psia	CS
48.	T-09 TCS/STC Reflux pot	D-02 Distillate	10 min. storage Vertical	5' diam. x 10' 55 psia	CS
49.	T-10 DCS/TCS Relux pot	D-03 Distillate	10 min. storage Vertical	4' diam. x 12' 320 psia	CS
50.	T-11 A, B Silane Shift Tanks	D-04 Distillate/ Feed to pyrolysis	4 hr. storage, each, Vertical	5' diam. x 9.4' 360 psia	316SS

TABLE 3.3-6 (Continued)

51.	T-13 Pyrolysis H_2 Receiver	H_2 Feed to Compressor	Vertical 25 psia	6' diam. x 12'	CS
52.	T-14 Lime Make-Up Tank	Lime solu. preparation	8 hr. storage Vertical, open	5' diam. x 9.2' 14.7 psia	CS
53.	T-15 Sludge Pump Tank	Sludge-solu. storage	4 hr. storage Vertical	5' diam. x 8'	316SS
54.	B-01 M. G. Silicon Storage Hopper	Feed to hydrogenation reactor	344 lb/hr Si	20' sq. x 5'/10' cone 14.7 psia	CS
55. & 56.	B-04 Pyrolysis Dust Bin	Solid residue	Small	3'diam. x 3' 25 psia	CS

FILTERS

57.	F-01 Crude TCS/STC Filter	In Line Filter	Small solic-liq.	50 gpm x 100μ	CS/316SS
58.	F-02 Waste Hydroxide Filter	Remove solid residues	100 gpm solid-liq.	Filtering area 67 ft.^{2}	CS/316SS
59.	F-03 Pyrolysis H_2 Filter	Remove solid residues	Small Bag solid-gas	20 ft.^{2} x 5μ	CS/cloth
60.	F-04 M. G. Silicon Unloading Filter	Solid-air separation in pneumatic conveyor	Small Bag solid-gas	20 ft.^{2} x 5μ	CS/cloth

TABLE 3.3-6 (Continued)

SOLID HANDLING EQUIPMENT

61.	S-01 M. G. Silicon Unloading Cyclone	Si feed transport	6" W. C. ΔP	417 ACFM	316SS
62.	S-02 Double Shell Blender	Si feed to reactor	Blending	20 ft.^{3}/shroud	304SS
63.	S-03 M. G. Silicon Lock Hopper	Si Feed to reactor	Locking	20 ft.^{3}	CS

UNCLASSED

64.	U-01 Quench Contactor Ejector	To withdraw gaseous products from reactor	6" W. C. Suction	100gpm 134 ACFM	316SS
65.	U-02 Lime Tank Agitator	Line solution preparation		3/4 HP	316SS
66.	U-03 Vent Gas Combustor	To burn vent gases from various units	20 ft.^{3}, [illegible].5 MM Btu/hr load	1.22 ACFM	316SS
67.	U-04 Vent Gas Ejector	To withdraw gases from combustion chamber	10" W. C. Suction	100gpm 1.0 CFM (STP)	316SS

PYROLYSIS SECTION (Primary)

68.	R-05 Silane Pyrolysis Reactors (six)	To convert silane to silicon	25 KW Power supply	3' diam., 15' tall, cone shape (approx.)	Monel/Quartz (pricing)
69.	X-01 Melters (six)	Melt silicon	60 KW Power supply		Graphite/Quartz, etc.

TABLE 3.3-6 (Continued)

70.	B-05 Powder Hoppers (six)	Pyrolysis Powder collection	96.1 lb/hr Si	8' diam. x 15' width cone bottom	316SS
71.	X-02 Hydrogen Cooler	Cool Hydrogen	42.4 lb/hr H_2	See Economic Analysis	CS/Other
72.	X-03 Hydrogen Blower	Blow Hydrogen	127 CFM (STP)	See Economic Analysis	CS/Other
73.	X-04 Dust Filter	Filter Dust	127 CFM (STP)	See Economic Analysis	CS/Other
74.	X-05 Star Valve (six)	Flow Control		See Economic Analysis	CS/Other
75.	X-06 Conveyor	Transport Material	96.1 lb/hr Si and its containers	See Economic Analysis	CS/Other
76.	X-07 Drum Loader	Load Drums		See Economic Analysis	

TABLE 3.3-7

PRODUCTION LABOR REQUIREMENTS FOR UCC SILANE PROCESS

Section/Unit Operation	Skilled Labor man-hr/KG Si (oper/shift)	Semiskilled Labor man-hr/KG Si (oper/shift)
1. Hydrogenation	0.00745 (1)	0.00745 (1)
2. Silane	0.02230 (3)	----
3. Pyrolysis	0.02980 (4)	----
4. Waste Treatment	0.00745 (1)	----
5. Hydrogen Compression	0.00745 (1)	----
TOTAL	0.0745 (10)	0.00745 (1)

Note

Manpower estimate for production labor requirements based on:

1. Dividing plant into sections
   - type of unit operation
   - mark off working area
2. Specify work duties required in each section
3. Estimate operators required to perform work duties in each section
   - type of unit operation
   - size of working area
   - degree of automation (batch, semi-continuous, continuous, etc.)

3.4 BCL Process for Silicon - Case A (Battelle Columbus Laboratories)

The chemical engineering analysis activity involves a preliminary process design of a plant to produce silicon via the technology under consideration.

The process flowsheet for the Case A of BCL process to manufacture silicon is shown in Figure 3.4-1. This process consists of several major processing operations of distillation, vaporization, stripping, condensation and a deposition reaction to produce silicon as well as electrolysis to recover the zinc.

Silicon tetrachloride ($SiCl_4$), which is the major raw material, is fed to the distillation section for purification, to remove impurities (such as boron and phosphorous). In the deposition section, purified silicon tetrachloride is vaporized and preheated to the reaction temperature, 927°C, before it is introduced into a silicon deposition unit, which is a fluidized bed reactor. Zinc vapor, produced by a specially designed induction-heated vaporizer, is also introduced to the reactor at the same temperature for the reaction. The reaction equation to show the silicon deposition is

$$SiCl_4 + 2Zn \rightarrow Si + 2ZnCl_2 \qquad (3.4\text{-}1)$$

Silicon granules produced by the deposition reaction, which descend to the bottom of reactor, are cooled and collected in containers. A small amount of silicon seed is fed to the reactor to control the particle size of the silicon product. Zinc chloride and unreacted zinc are recovered and fed to the electrolysis section, while unreacted silicon tetrachloride is recycled to the distillation section.

In the electrolysis section, zinc chloride is reduced to zinc by low voltage (4-5 volts) electrolysis cells. Zinc is recycled to the deposition unit, while chlorine gas is collected as the by-product. The deposition and electrolysis sections are purged with inert gas (such as argon). Waste gases from various sections are collected and treated with hydrate lime solution in the waste treatment section.

A process design was performed to obtain data for a cost analysis of a plant to produce silicon by this new technology. The design was based on a plant to produce 1000 metric tons/yr of silicon via the BCL process. In Case A, two deposition reactors and six electrolysis cells are required.

The detailed status sheet for the process design package is shown in Table 3.4-1 and is representative of the various sub-items that make up the activity. 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:

- Process Flowsheet-----------------Figure 3.4-1
- Base Case Conditions--------------Table 3.4-2
- Reaction Chemistry----------------Table 3.4-3
- Raw Material Requirements---------Table 3.4-4
- Utility Requirements--------------Table 3.4-5
- Major Process Equipment-----------Table 3.4-6
- Production Labor Requirements----Table 3.4-7

The process design provides detailed data for raw materials, utilities, major process equipment and production labor requirements which are necessary for polysilicon production.

TABLE 3.4-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR BCL PROCESS – Case A

	Prel. Process Design Activity	Status
1.	Specify Base Case Conditions	●
	1. Plant Size	●
	2. Product Specifics	●
	3. Additional Conditions	●
2.	Define Reaction Chemistry	●
	1. Reactants, Products	●
	2. Equilibrium	●
3.	Process Flow Diagram	●
	1. Flow Sequence, Unit Operations	●
	2. Process Conditions (T, P, etc.)	●
	3. Environmental	●
	4. Company Interaction (Technology Exchange)	●
4.	Material Balance Calculations	●
	1. Raw Materials	●
	2. Products	●
	3. By-Products	●
5.	Energy Balance Calculations	●
	1. Heating	●
	2. Cooling	●
	3. Additional	●
6.	Property Data	●
	1. Physical	●
	2. Thermodynamic	●
	3. Additional	●

	Prel. Process Design Activity	Status
7.	Equipment Design Calculations	●
	1. Storage Vessels	●
	2. Unit Operations Equipment	●
	3. Process Data (P, T, rate, etc.)	●
	4. Additional	●
8.	List of Major Process Equipment	●
	1. Size	●
	2. Type	●
	3. Materials of Construction	●
8a.	Major Technical Factors	●
	(Potential Problem Areas)	●
	1. Materials Compatibility	●
	2. Process Conditions Limitations	●
	3. Additional	●
9.	Production Labor Requirements	●
	1. Process Technology	●
	2. Production Volume	●
10.	Forward for Economic Analysis	●

○ Plan
◐ In Progress
● Complete

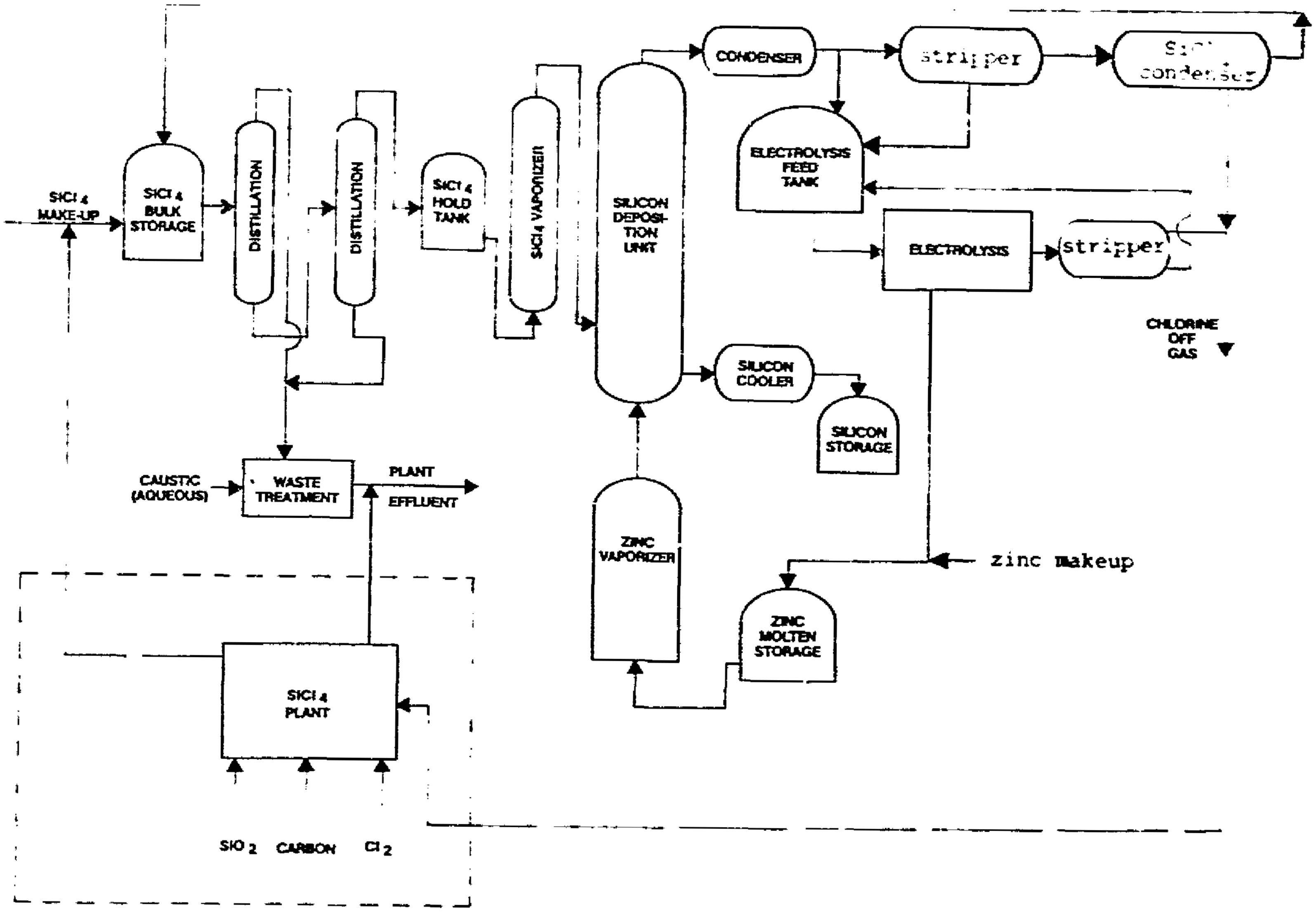


Figure 3.4-1 Process Flow Sheet for BCL Process-Case A

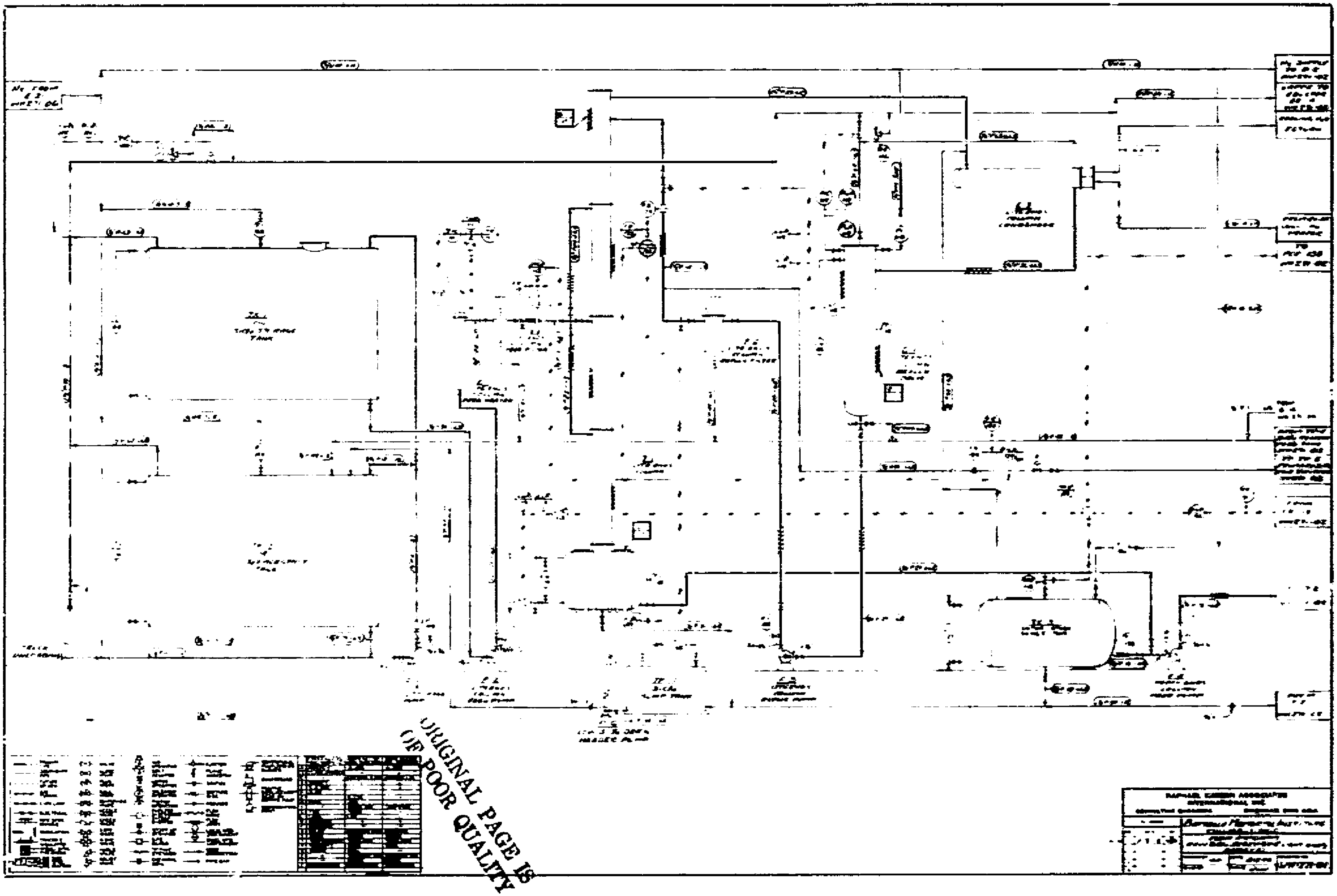


Figure 3.4-2 Process Flow Sheet for BCL Process-Case A

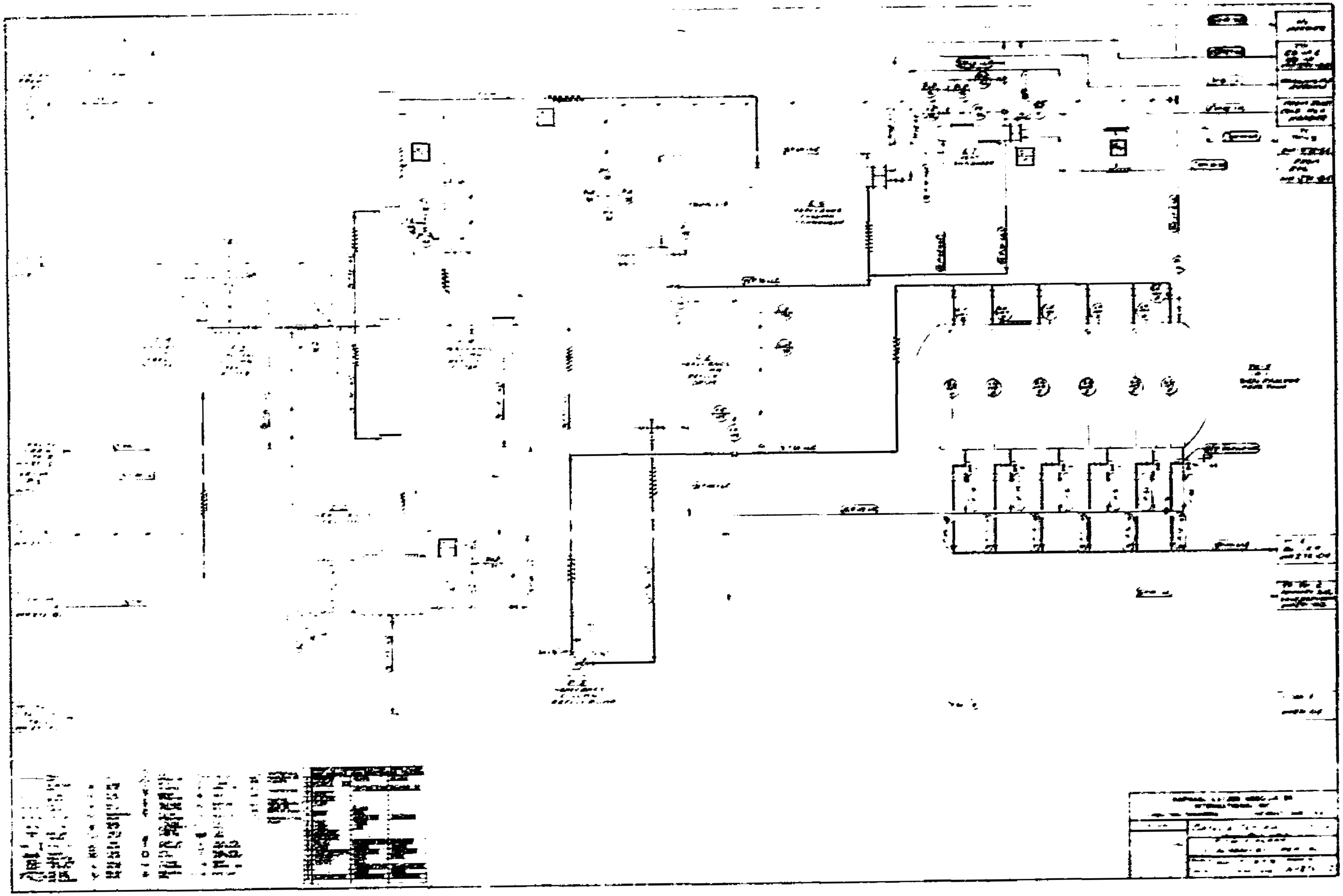


Figure 3.4-2 (Continued)

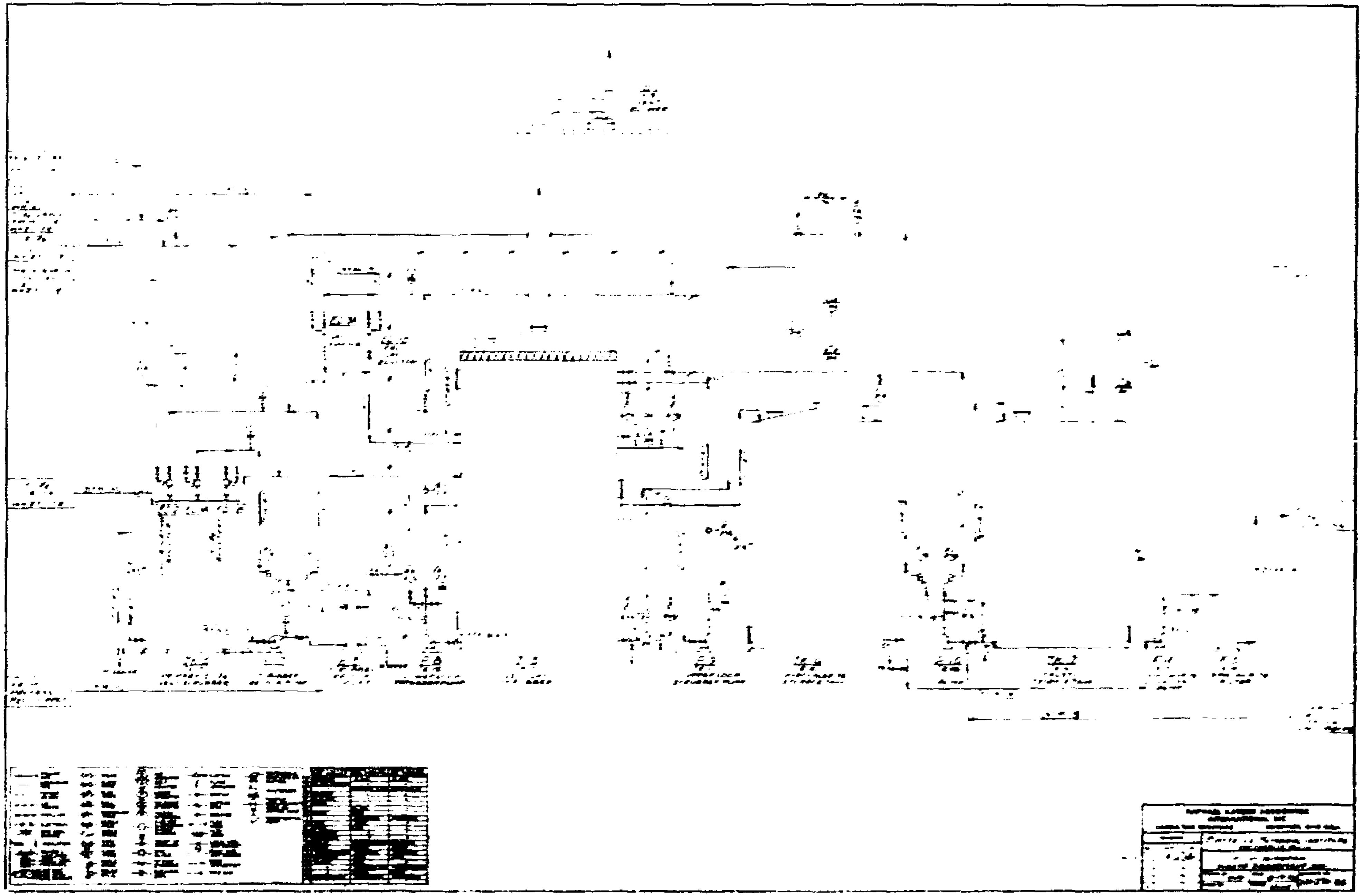


Figure 3.4-2 (Continued)

Note: For 50 MT/yr
Facility only

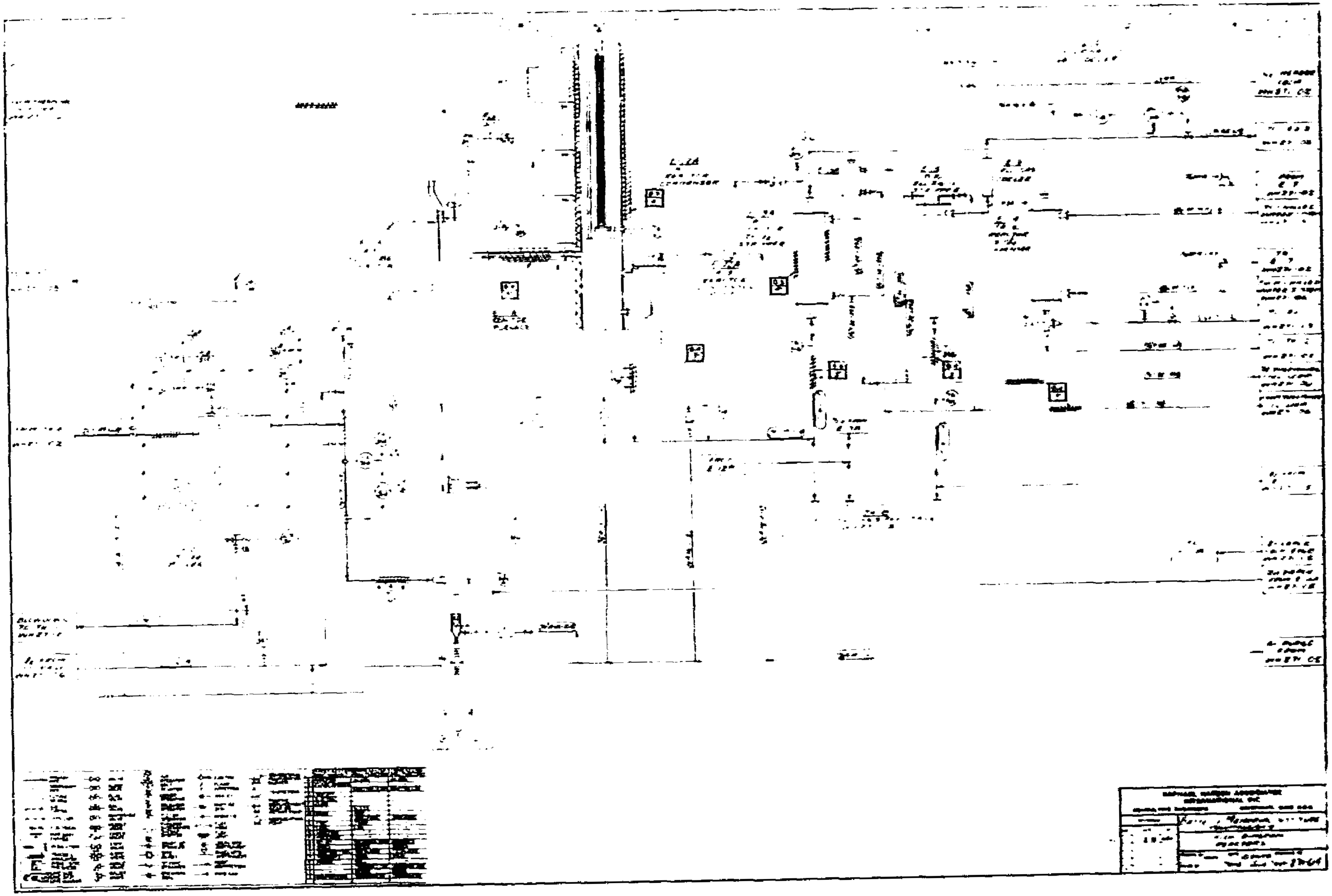


Figure 3.4-2 (Continued)

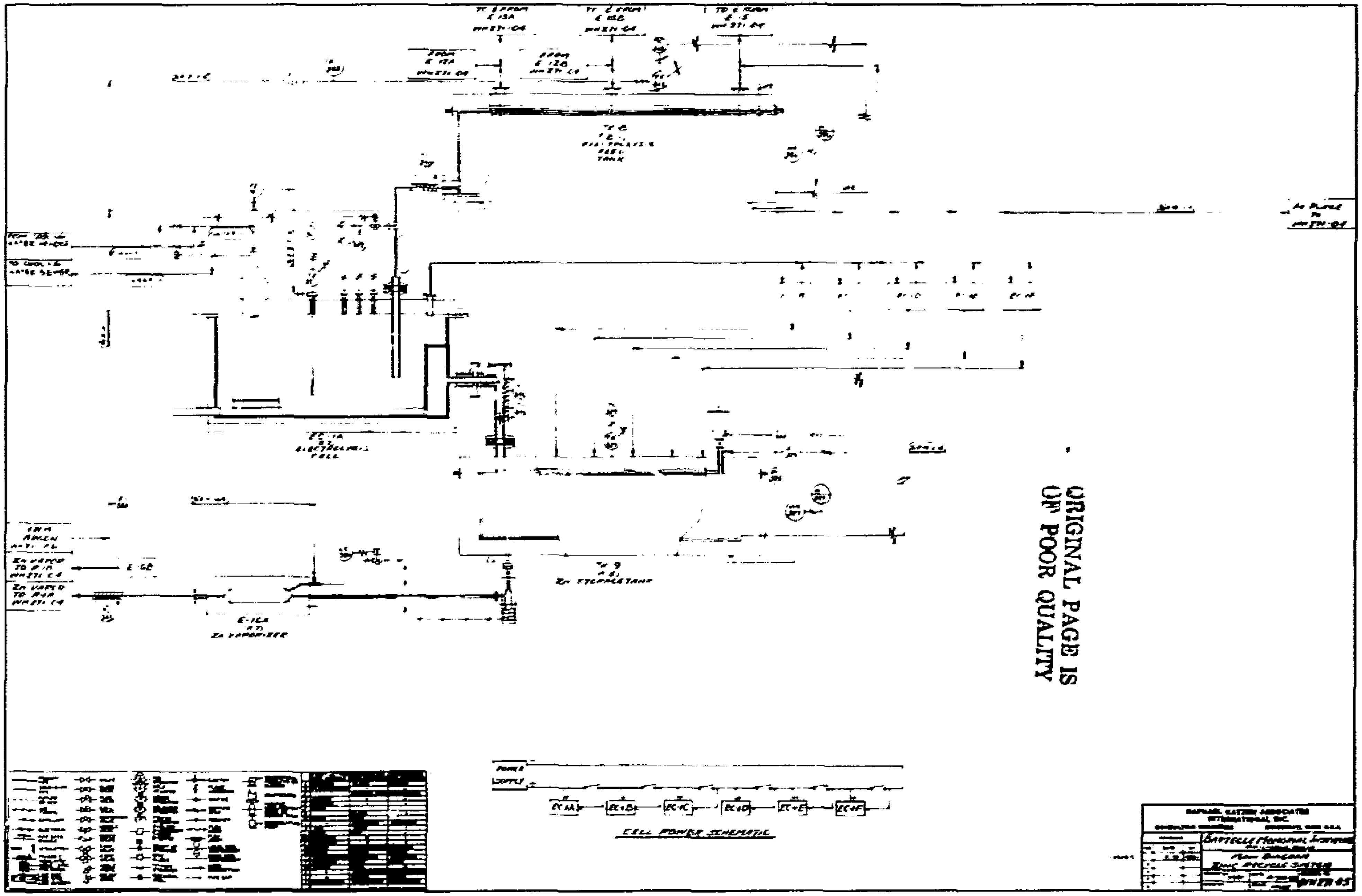


Figure 3.4-2 (Continued)

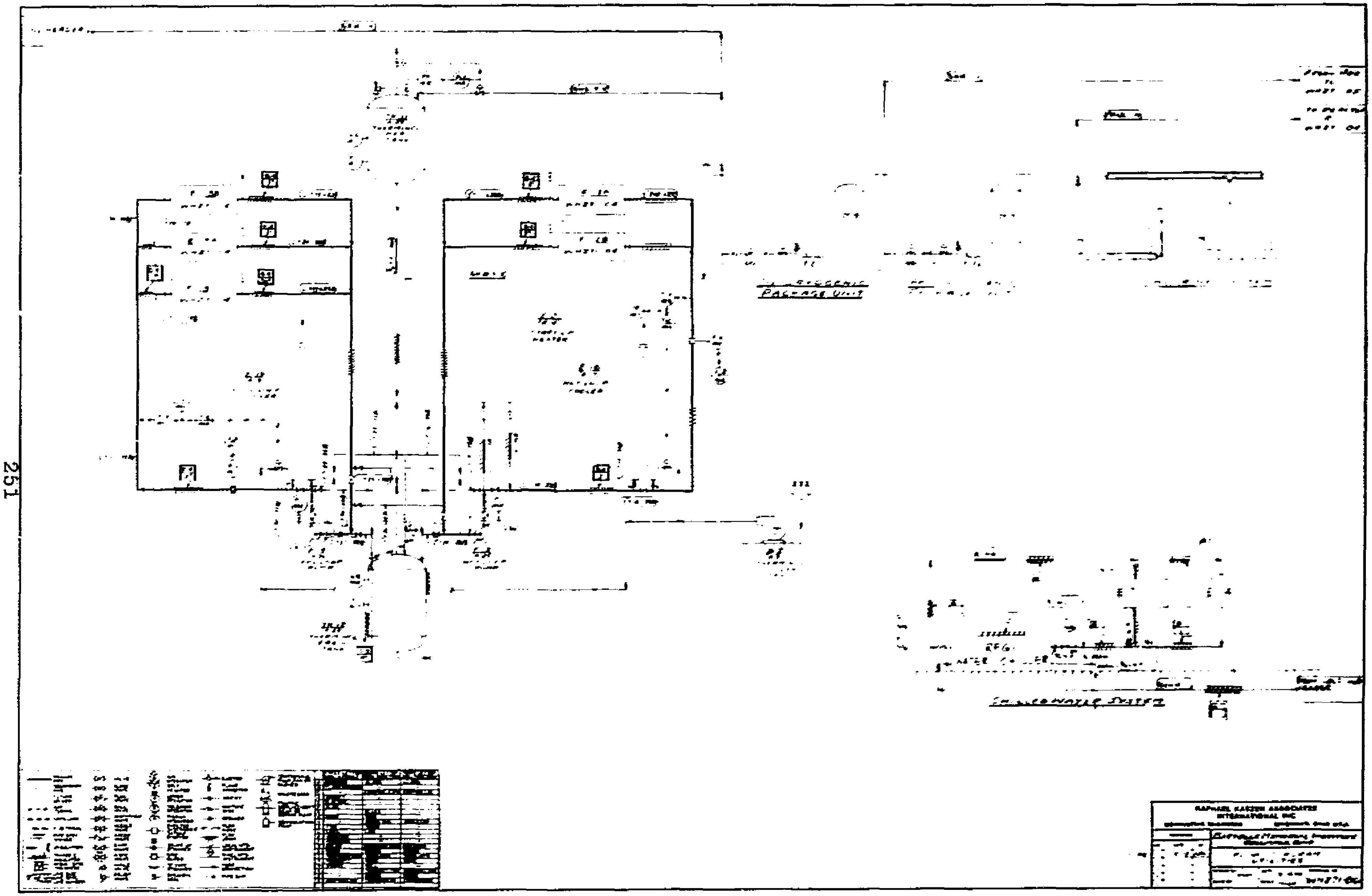
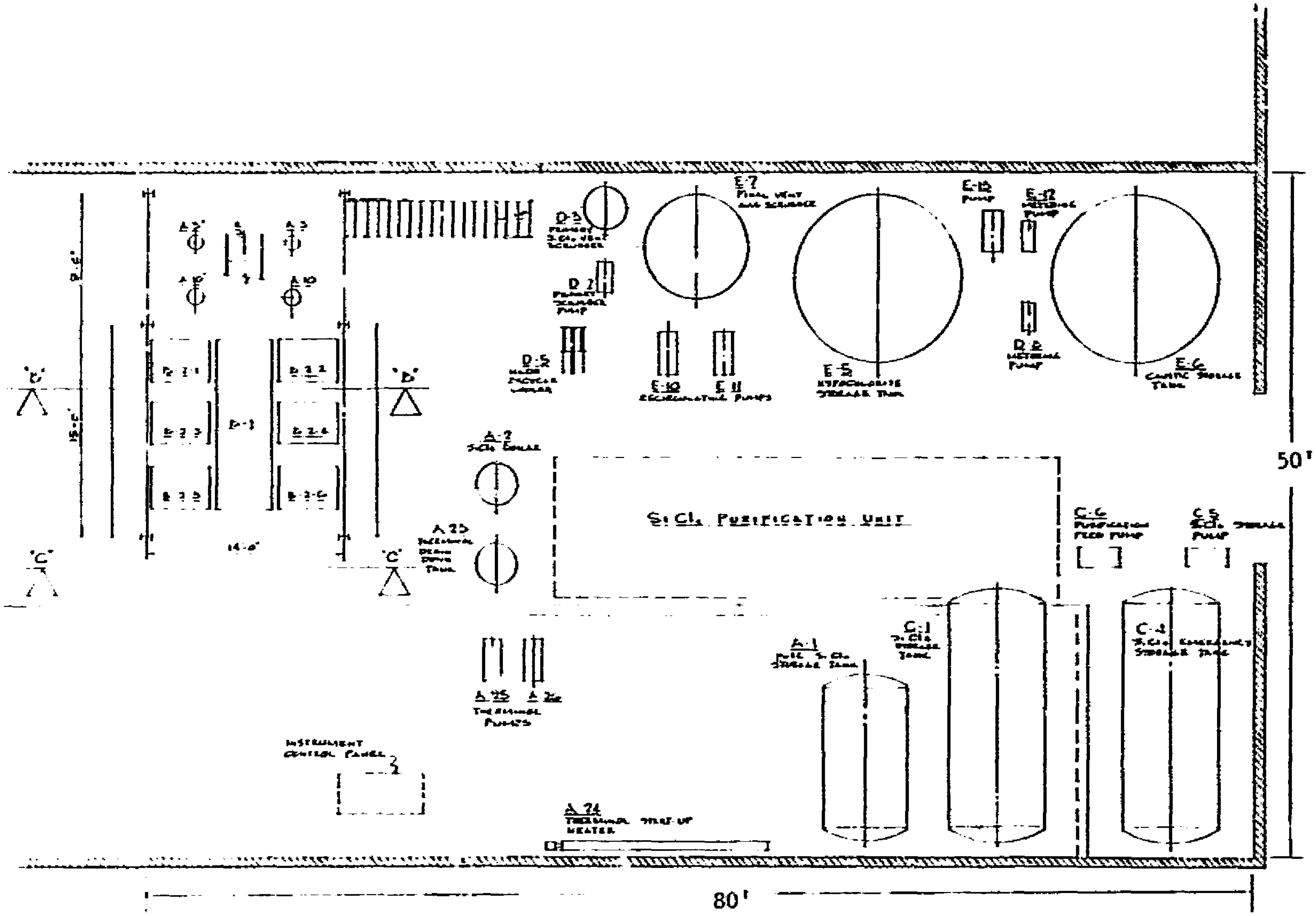


Figure 3.4-2 (Continued)



PLOT PLAN

Figure 3.4-2 (Continued)

TABLE 3.4-2
BASE CASE CONDITIONS FOR BCL PROCESS - Case A

1. Plant Size
-silicon produced from silicon tetrachloride (TET)
-1000 metric tons/yr of silicon
-solar cell grade silicon
-solid phase product form (granules)
2. Light End Distillation
-purification of TET by distillation
-remove 4% chlorosilanes as the light end
-80°C, 10 psig

3. Heavy End Distillation
-purification of TET by distillation
-remove 4% impurities as the heavy end
-92% over-all yield of TET from both distillations
-80°C, 10 psig

4. TET Vaporizer
-to supply TET vapor for deposition reactor
-by power input (resistance heater)
-hold at constant level and constant pressure
-164°F

5. Deposition Reactor
-reduce TET by zinc to produce silicon
-deposit on pure silicon seed
-fluid bed
-927°C (1700°F, 1 atm)
-63% conversion of TET to silicon

6. Reactor Condenser
-to condense gases from reactor ($ZnCl_2$, unreacted Zn and $SiCl_4$ gases)
-partial condensation
-using therminol 66 as the coolant
-927°C inlet temperature and 350°C outlet temperature

7. Reactor $ZnCl_2$ Stripper
-work as partial condenser
-to condense $ZnCl_2$gas from $SiCl_4$ gas
-operating at the temperature right above $ZnCl_2$ melting point (318°C), 350°C
-using therminol 66 as the coolant

, Cell $ZnCl_2$ Stripper
-operates as partial condenser
-to condense $ZnCl_2$ gas from Cl_2 and $SiCl_4$ gases
-operating at the temperature right above $ZnCl_2$ melting point (318°C), 350°C
-using therminol 66 as the heat exchange medium

TABLE 3.4-2 (Continued)

9. Reactor $SiCl_4$ Condenser
   -condense $SiCl_4$ gas for recycle
   -antifreeze as the coolant
   -350°C inlet temperature, 20°F outlet temperature.

10. Electrolysis
    -electrolytic recovery of Zn from $ZnCl_2$
    -Cl_2 gas is by product
    -95% Zn recovery
    -500°C, approx. 1 atm

11. Zinc Vaporizer
    -to vaporize Zinc
    -by induction heating
    -927°C, approx. 1 atm.

12. Wastes Treatment
    -to scrub and neutralize $SiCl_4$ and chlorosilane gases
    -caustic solution used to neutralize

13. Operating Ratio
    -approximately 80% utilization (on stream time)
    -approximately 7,000 hr/yr production

14. Storage Considerations
    -feed material (two week supply)
    -product (two shifts storage)
    -process (several hours)

TABLE 3.4-3
REACTION CHEMISTRY FOR BCL PROCESS - Case A

1. Silicon Deposition

$2Zn + SiCl_4 \rightarrow Si\downarrow + 2ZnCl_2$

2. Electrolysis

$ZnCl_2 \xrightarrow{electroly.} Zn(l) + Cl_2\ (g)$

3. Waste Treatment

$SiCl_4 + 2H_2O \xrightarrow{aq} SiO_2 + 4HCl(aq)$

$NaOH(aq) + HCl(aq) \rightarrow NaCl(aq) + H_2O$

or

$Ca(OH)_2(aq) + 2HCl(aq) \rightarrow CaCl_2(aq) + 2H_2O$

3a. Waste Treatment (50 MT/yr unit)

$Cl_2(g) + 2NaOH(aq) \rightarrow NaOCl(aq) + NaCl(aq) + H_2O$

Table 3.4-4

Raw Material Requirements for BCL Process - Case A

	Raw Material	Requirements lb/KG of Silicon
1.	Silicon Tetrachloride, $SiCl_4$	15.68[1]
2.	Zinc, Zn	0.54
3.	Caustic (50%), NaOH(aq)	5.23
	or	
	Lime (99%), $Ca(OH)_2$	2.85[2]
4.	Argon	3.1 SCF[3]
5.	Nitrogen	7.6 SCF[3]
6.	Chlorine, Cl_2 (by-product)	11.12

---

1. Includes light wastes (4%), heavey wastes (4%) and additional losses (7%).

2. Includes neutralization of distillation section, deposition section, electrolysis section and chlorination losses.

3. Estimate from BCL

TABLE 3.4-5

UTILITY REQUIREMENTS FOR BCL PROCESS - Case A

Utility/Function		Requirements/Kg of Silicon Product
1. Electricity		30.92 kw-hr
1. Low Volatage D.C. for Electrolysis	(20.51)	
2. Zinc Vaporizer Induction Heated	(5.62)	
3. Preheat Section of Deposition Unit Induction Heated	(1.39)	
4. Electrolysis Feed Tank Heater	(0.24)	
5. Molten Zinc Storage Heater	(0.10)	
6. $SiCl_4$ Vaporizer	(0.53)	
7. Pumps, Blowers	(2.53)	
2. Steam (50 PSIA)		9.67 pounds
1. #1 Purification Column Reboiler	(4.59)	
2. #2 Purification Column Reboiler	(4.30	
3. Caustic Storage Heating	(0.29)	
4. #1 Purification Column Preheater	(0.49)	
3. Cooling Water		37.88 Gallons
1. #1 Purification Column Condenser	(16.94)	
2. #2 Purification Column Condenser	(15.88)	
3. Purified Tet Cooler	(1.67)	
4. Chlorination Cooler (H-17)	(0.53)	
5. Cell Gas Cooler (H-18)	(2.86)	
4. Process Water		24.20 Gallons
1. Diluent for Waste Treatment	(24.20)	
5. Refrigeration		2.38 kBtu
1. Reactor $SiCl_4$ Condenser (H-11)	(1.28)	
2. $SiCl_4$ Vent Condenser (H-07)	(1.10)	

Note: k = kilo = 10^3

TABLE 3.4-6

LIST OF MAJOR PROCESS EQUIPMENT
FOR BCL – Case A

	Equipment	Function	Size/Type	Material of Construction	Capacity Ratio to 1000 MT/yr
PROCESS TOWER AND INTERNALS					
1.	D-01 Light End Distillation Column	To purify $SiCl_4$	8" dia. x 21', packed 13.5'	Column, CS/packing, SS	20
2.	D-02 Heavy End Distillation Column	To purify $SiCl_4$	8" dia. x 21', packed 13.5'	Column, CS/packing, SS	20
3.	A-01 Primary $SiCl_4$ Vent Scrubber	To scrub $SiCl_4$ vent gas	3' dia. x 4'4" T/T, 225 gal/flat bottom	FRP	1
4.	A-02 Final $SiCl_4$ Vent Scrubber	To scrub $SiCl_4$ vent gas	7'6" dia. x 17'4" T/T/ 4 pp trays, Teflon dimister	FRP	1
HEAT EXCHANGER					
5.	H-01 L.E. Column Feed Heater	To preheat feed to D-01	2' dia. x 5', 15,013 Btu/hr / external heater	CS	20
6.	H-02 L.E. Column Reboiler	Reboiler of D-01	2' dia. x 3', 51,522 Btu/hr / external heater	CS	20
7.	H-03 L.E. Column Condenser	Total condenser of D-01	47,430 Btu/hr/shell-tube H.E.	CS	20
8.	H-04 H.E. Column Feed Heater	To preheat feed to D-02	2' dia. x 5', 14,331 Btu/hr/external heater	CS	20

TABLE 3.4-6 (Continued)

9.	H-05 H.E. Column Reboiler	Reboiler of D-02	2' dia. x 3', 56,641 Btu/hr/external heater	CS	20
10.	H-06 H.E. Column Condenser	Total condenser of D-02	52,292 Btu/hr/shell-tube H.E.	CS	20
11.	H-07 $SiCl_4$ Vent Condenser	Condense $SiCl_4$ from vent gas	38 ft^2, 18,000 Btu/hr/shell-tube H.E.	CS	20
12.	H-08 $SiCl_4$ Vaporizer	To provide $SiCl_4$ vapor to reactor	2.75' dia. x 3' T/T. 13,648 Btu/hr/resistance heater	CS	20
13.	H-09 Reactor Condenser	To condense by products from reactor	14" dia. x 6.4', 126,237.2 Btu/hr	Graphite W/SS shell	20
14.	H-10 Reactor $ZnCl_2$ Stripper	To condense $ZnCl_2$ gas	12 ft^2, 2,652 Btu/hr/shell-tube H.E., finned U-tube	316 SS	20
15.	H-11 $SiCl_4$ Condenser	To condense $SiCl_4$ gas for recycle	6,401 Btu/hr (x 4.62 = 29.573 Btu/hr)	316 SS	20
16.	H-12 Cell $ZnCl_2$ Stripper	To condense $ZnCl_2$ vapor	9,841.4 Btu/hr/shell-tube, H.E. (x 0.32)	Inconel 600	20
17.	H-13 Therminol Cooler (cold circuit)	To cool Therminol 66	68 ft^2, 11,000 Btu/hr/shell-tube H.E., 500 psia	CS	20
18.	H-14 Therminol Cooler (hot circuit)	To cool Therminol 66	262 ft^2, 120,000 Btu/hr/shell-tube H.E., 500 psia	CS	20
19.	H-15 Start-up Heater	Therminol start up heater	98,950 Btu/hr/U-tube 15', resistance heater	CS	20
20.	H-16 Silicon Product Cooler (two)	To cool the Si product from reactor	5,735 Btu/hr	SiC	20

TABLE 3.4-6 (Continued)

20a.	H-17 Chlorination Cooler		20,000 Btu/hr, Area 200 ft^2	SS	1
20b.	H-18 Cell Gas Cooler		1.08 x 10^5 Btu/hr, Area 1805 ft^2	CS	1

PROCESS AND STORAGE VESSELS

21.	T-01 $SiCl_4$ Storage Tank	Storage/feed to purification	7' dia. x 16' T/T/ 4,600 gal	CS	20
22.	T-02 $SiCl_4$ Emergency Storage Tank	Storage/feed to purification	7' dia. x 16' T/T/ 4,600 gal	CS	20
23.	T-03 L.E. Column Reflux Drum	To hold distillate for reflux	12" dia. x 4'/23 gal	CS	20
24.	T-04 Surge Tank	Surge Tank for D-01 bottom	3' dia. x 4'/200 gal	CS	20
25.	T-05 Sump Tank	Sump for purification unit	3' dia. x 4'/200 gal	CS	20
26.	T-06 H.E. Column Reflux Drum	To hold distillate for reflux	12" dia. x 4'/23 gal	CS	20
27.	T-07 Pure $SiCl_4$ Storage Tank	Storage/feed to $SiCl_4$ Vaporizer	6' dia. x 10' T/T/ 1900 gal	CS	20
28.	T-08 Electrolysis Feed Tank	Storage feed $ZnCl_2$ to electrolysis cell	50" x 158" x 38"H/ 7" graphite TH	Graphite/304 SS	20
29.	T-09 Molter Zinc Storage Tank	Storage/feed to Zinc vaporizer	W/heater 68,242 Btu/hr	Graphite/304 SS	20
30.	T-10 Therminol Head Tank	Storage Therminol	1.5' dia. x 3.75' T/T/ 49.6 gal	CS	20

TABLE 3.4-6 (Continued)

31.	T-11 Therminol Drain Down Tank	To store drained Therminol	2.75' dia. x 3' T/T/ 133 gal	CS	20
32.	T-12 Chlorine Supply Tank	To supply chlorine gas	1 1/2' dia. x 3'/ 37.62 gal	CS	20
33.	T-13 Lime Storage Tank	Storage Lime	12' dia. x 14'6" T/T/ 12,000 gal	FRP	1

PUMPS WITH DRIVERS

34.	P-01 Purification Feed Pump	To feed $SiCl_4$ to storage tank	30 gpm, 31' head/ centrifugal, 1 1/2 hp	CS	20
35.	P-02 L.E. Column Feed Pump	To supply $SiCl_4$ to preheater	28.9 gph, Δp = 72 psia/ 0.5 hp.	CS	20
36.	P-03 L.E. Column Relux Pump	D-01 Reflux	51.7 gph, Δp = 23 psia/ 0.5 hp.	CS	20
37.	P-04 Surge Tank Pump	To supply $SiCl_4$ to H.E. Column	29.4 gph, Δp = 53 psia/ 0.5 hp.	CS	20
38.	P-05 Sump Pump	To pump $Sicl_4$ to emergency tank	30 gpm, 31' head/ centrifugal, 1 1/2 hp.	CS	20
39.	P-06 L.E. Column Bottom Pump	To pump $SiCl_4$ to surge tank	29.4 gph, Δp = 53 psia/ 0.5 hp.	CS	20
40.	P-07 H.E. Column Relux Pump	D-02 Reflux	57.1 gph, [illegible] 25 psia/ 0.5 hp.	CS	20
41.	P-08 H.E. Column Bottom Pump	To pump bottom solution to waste treatment	1.3 gph, Δp = 25 psia/ 0.5 hp.	CS	20
42	P-09 $SiCl_4$ Vaporizer Feed Pump	To feed $SiCl_4$ to Vaporizer	15 gph, 31' head/ 1/2 hp	CS	20

TABLE 3.4-6 (Continued)

43.	P-10 Reactor Condenser Circulating Pump	To circulate condensates	2.4 gpm, 30' head/1/2 hp	Graphite	20
44.	P-11 Cold Circuit Pump (two)	Cold Therminol circulation	20 gpm, 85' head/centrifugal, 2 hp.	CS	20
45.	P-12 Hot Circuit Pump	Hot Therminol circulation	62 gpm, 85' head/centrifugal, 4 hp.	CS	20
46.	P-13 Primary Scrubber Recirculation Pump	Recirculation for Scrubber A-01	20 gpm, 125' head/ centrigugal, 2.5 hp.	Duriron	1
47	P-14 Primary Scrubber Lower-loop Recirculating Pump	Circulate solution for Lower-loop of Scrubber A-02	100 gpm, 103' head/ centrifugal, 7 1/2 hp.	Duriron	1
48	P-15 Primary Scrubber Upper-loop Recirculating Pump	Circulate solution for upper-loop of Scrubber A-02	100 gpm, 13' head/ centrifugal, 2 hp.	Duriron	1
49.	P-16 Make up Lime Metering Pump	Lime make up	0.9 gpm, 25' head/ centrifugal, 1/2 hp.	CS	1

FILTERS

50.	F-01 L.E. Column Feed Filter	Remove solids	29 gph, Δp = 5 psia/ 140 micron	CS	20
51.	F-02 L.E. Column Reflux Filter	Remove solids	30 gph, Δp = 5 psia/ 140 micron	CS	20
52.	F-03 H. E. Column Feed Filter	Remove solids	52 gph, Δp = 5 psia/ 140 micron	CS	20
53.	F-04 H.E. Column Relfux Filter	Remove solids	31 gph, Δp = 5 psia/ 140 micron	CS	20

TABLE 3.4-6 (Continued)

54.	F-05 Therminol Cooler Blower Filter	To filter the solids from air			20

SPECIALIZED EQUIPMENTS

55.	R-01 Fluidized Bed Reactor (two)	To reduce $SiCl_4$ to Si by Zn	1330.2 Btu/hr, 6.5" dia.	Graphite Lined /SS	20
56.	FN-01 Furnace (two)	To preheat $SiCl_4$ gas	272,966 Btu/hr		20
57.	B-01 Seed Addition Hopper (two)	To feed Si seed to the reactor		310 SS	20
58.	B-02 Si Product Hopper (four)	To hold Si product	6 gal	310 SS	20
59.	B-03 Zinc Hopper	To hold make up Zinc	40 gal	CS	20
60.	C-01 Therminol Cooler Blower	Therminol system air cooler blower	500 acfm fan/electric, 1 1/2 hp., 12-1/2" wheel	CS	20
61.	C-02 Scrubber Vent Blower	Suck $SiCl_4$ gas for A-01 & A-02	10,000 acfm/electric, 30 hp. 31-1/2" wheel	FRP	1
62.	E-01 Eductor (two)	$SiCl_4$ scrubbing (Scrubber D-05)	20 gpm, Δp = 47.4 psia/ Hydraulic ejector, 1-1/2" NPT	P.V.C.	1
63.	EC-01 Electrolysis Cell (six)	To recover Zn from $ZnCl_2$	5,000 ~6,000 amp cells	Graphite/SS	20
64.	PW-01 Power Supply	To supply power to electrolysis cell	545,933 Btu/hr.		20
65.	VP-01 Zinc Vaporizer (two)	To provide zinc vapor to reactor	104,128.8 Btu/hr 13.5" dia. x 32"	Quartz	20

TABLE 3.4-6 (Continued)

NOTE:

1. For the 1000 MT/yr plant, items 3, 4, 33, 46, 47, 48, 49, 61, and 62 are used for waste treatment of distillation wastes (light, heavy) and vent gases.
2. In the 50 MT/yr facility, these items are used for hypochlorite maufacture which is not present in the 1000 MT/yr plant.
3. For H-11, the operation conditions were changed from 171°F - 32°F to 662°F - 20°F.
4. For H-12, the operations conditions have been chnaged from ΔT = 855°F to 270°F.

TABLE 3.4-7

PRODUCTION LABOR REQUIREMENTS FOR BCL PROCESS - Case A

	Section		Labor man-hr/KG Si (oper/shift)
1.	Purification	(I)	0.01402 (2)
2.	Deposition	(II)	0.01402 (2)
3.	Electrolysis	(III)	0.02103 (3)
4.	Waste Treatment	(IV)	0.00701 (1)
5.	Product Handling	(V)	0.00701 (1)
		TOTAL	0.06309 (9)

Note

Manpower estimate for production labor requirements based on:

1. Dividing plant into sections
   - -type of unit operation
   - -mark off working area
2. Specify work duties required in each section
3. Estimate operators required to perform work duties in each section
   - -type of unit operation
   - -size of working area
   - -degree of automation (batch, semi-continuous, continuous, etc.)

3.5 BCL Process for Silicon - Case B (Battelle Columbus Laboratories)

The chemical engineering analysis activity involves a preliminary process design of a plant to produce silicon via the technology under consideration.

The process flowsheet for the Case B of the BCL process to manufacture silicon is shown in Figure 3.5-1. This process consists of several major processing operations of distllation, vaporization, strippping, condensation and a deposition reaction to produce silicon as well as elecrolysis to recover the zinc.

Silicon tetrachloride ($SiCl_4$), which is the major raw material, is fed to the distillation section for purification, to remove impurities (such as boron and phosphorous). In the deposition section, purified silicon tetrachloride is vaporized and preheated to the reaction temperature, 927°C, before it is introduced into a silicon deposition unit, which is a fluidized bed reactor. Zinc vapor produced by a specially designed induction-heated vaporizer is also introduced to the reactor at the same temperature for the reaction. The reaction equation to show the silicon deposition is

$$SiCl_4 + 2Zn \rightarrow Si + 2ZnCl_2 \qquad (3.5-1)$$

Silicon granules produced by the deposition reaction, which descend to the bottom of reactor, are cooled and collected in containers. A small amount of silicon seed is fed to the reactor to control the particle size of the silicon product. Zinc chloride and unreacted zinc are recovered and fed to the electrolysis section, while unreacted silicon tetrachloride is recycled to the distillation section.

In the electrolysis section, zinc chloride is reduced to zinc by low voltage (4-5 volts) electrolysis cells. Zinc is recycled to the deposition unit, while chlorine gas is collected as the by-product. The deposition and electrolysis sections are purged with inert gas (such as argon). Waste gases from various sections are collected and treated with hydrate lime solution in the waste treatment section.

A process design was performed to obtain data for a cost analysis of a plant to produce silicon by this new technology. The design was based on a plant to produce 1000 metric tons/yr of silicon via the BCL process. In case B, the process contains one deposition reactor and two electrolysis cells as compared with two deposition reactors and six electrolysis cells for Case A which was reported earlier.

The detailed status sheet for the process design package is shown in TAble 3.5-1 and is representative of the various sub-items that make up the activity. 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:

- Base Case Conditions------------------Table 3.5-2
- Reaction Chemistry--------------------Table 3.5-3
- Raw Material Requirements-------------Table 3.5-4
- Utility Requirements------------------Table 3.5-5
- Major Process Equipment---------------Table 3.5-6
- Production Labor Requirements---------Table 3.5-7

The process design provides detailed data for raw materials, utilities, major process equipment and production labor requirements which are necessary for polysilicon production.

TABLE 3.5-1 CHEMICAL ENGINEERING ANALYSES:
PRELIMINARY PROCESS DESIGN ACTIVITIES FOR BCL Process (Case B)

Prel. Process Design Activity	Status
1. Specify Base Case Conditions	●
1. Plant Size	●
2. Product Specifics	●
3. Additional Conditions	●
2. Define Reaction Chemistry	●
1. Reactants, Products	●
2. Equilibrium	●
3. Process Flow Diagram	●
1. Flow Sequence, Unit Operations	●
2. Process Conditions (T, P, etc.)	●
3. Environmental	●
4 Company Interaction (Technology Exchange)	●
4. Material Balance Calculations	●
1. Raw Materials	●
2. Products	●
3. By-Products	●
5. Energy Balance Calculations	●
1. Heating	●
2. Cooling	●
3. Additional	●
6. Property Data	●
1. Physical	●
2. Thermodynamic	●
3. Additional	●

Prel. Process Design Activity	Status
7. Equipment Design Calculations	●
1. Storage Vessels	●
2. Unit Operations Equipment	●
3. Process Data (P, T, rate, etc.)	●
4. Additional	●
8. List of Major Process Equipment	●
1. Size	●
2. Type	●
3. Materials of Construction	●
8a. Major Technical Factors	●
(Potential Problem Areas)	●
1. Materials Compatibility	●
2. Process Conditions Limitations	●
3. Additional	●
9. Production Labor Requirements	●
1. Process Technology	●
2. Production Volume	●
10. Forward for Economic Analysis	●

O Plan
◐ In Progress
● Complete

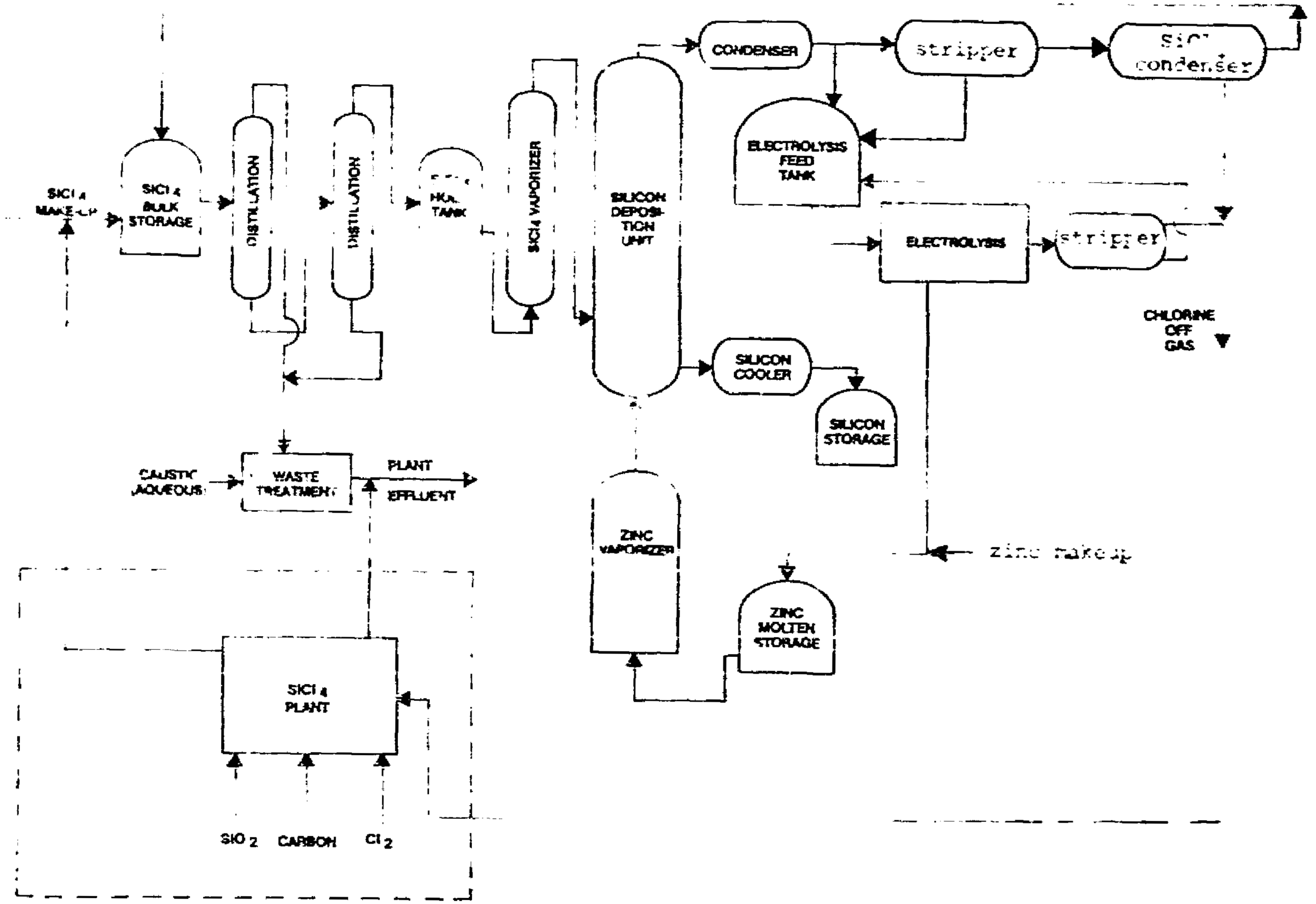


Figure 3.5-1 Process Flow Sheet for BCL Process - Case B

TABLE 3.5-2
BASE CASE CONDITIONS FOR BCL PROCESS (Case B)

1. Plant Size
   - -silicon produced from silicon tetrachloride (TET)
   - -1000 metric tons/yr of silicon
   - -solar cell grade silicon
   - -solid phase product form (granules)
2. Light End Distillation
   - -purification of TET by distillation
   - -remove 4% chlorosilanes as the light end
   - -80°C, 10 psig

3. Heavy End Distillation
   - -purification of TET by distillation
   - -remove 4% impurities as the heavy end
   - -92% over-all yield of TET from both distillations
   - -80°C, 10 psig

4. TET Vaporizer
   - -to supply TET vapor for deposition reactor
   - -by power input (resistance heater)
   - -hold at constant level and constant pressure
   - -164°F

5. Deposition Reactor
   - -reduce TET by zinc to produce silicon
   - -deposit on pure silicon seed
   - -fluid bed
   - -927°C (1700°F, 1 atm)
   - -63% conversion of TET to silicon

6. Reactor Condenser
   - -to condense gases from reactor ($ZnCl_2$, unreacted Zn and $SiCl_4$ gases)
   - -partial condensation
   - -using therminol 66 as the coolant
   - -927°C inlet temperature and 350°C outlet temperature

7. Reactor $ZnCl_2$ Stripper
   - -work as partial condenser
   - -to condense $ZnCl_2$ gas from $SiCl_4$ gas
   - -operating at the temperature right above $ZnCl_2$ melting point (318°C), 350°C
   - -using therminol 66 as the coolant

8. Cell $ZnCl_2$ Stripper
   - -operates as partial condenser
   - -to condense $ZnCl_2$ gas from Cl_2 and $SiCl_4$ gases
   - -operating at the temperature right above $ZnCl_2$ melting point (318°C), 350°C
   - -using therminol 66 as the heat exchange medium

TABLE 3.5-2 (Continued)

9. Reactor $SiCl_4$ Condenser
   - condense $SiCl_4$ gas for recycle
   - antifreeze as the coolant
   - 350°C inlet temperature, 20°F outlet temperature.

10. Electrolysis
    - electrolytic recovery of Zn from $ZnCl_2$
    - Cl_2 gas is by product
    - 95% Zn recovery
    - 500°C, approx. 1 atm

11. Zinc Vaporizer
    - to vaporize Zinc
    - by induction heating
    - 927°C, approx. 1 atm.

12. Wastes Treatment
    - to scrub and neutralize $SiCl_4$ and chlorosilane gases
    - caustic solution used to neutralize

13. Operating Ratio
    - approximately 80% utilization (on stream time)
    - approximately 7,000 hr/yr production

14. Storage Considerations
    - feed material (two week supply)
    - product (two shifts storage)
    - process (several hours)

TABLE 3.5-3
REACTION CHEMISTRY FOR BCL PROCESS (Case B)

1. **Silicon Deposition**

   $2Zn + SiCl_4 \rightarrow Si\downarrow + 2ZnCl_2$

2. **Electrolysis**

   $ZnCl_2 \xrightarrow{\text{electroly.}} Zn(l) + Cl_2\ (g)$

3. **Waste Treatment**

   $SiCl_4 + 2H_2O \xrightarrow{aq} SiO_2 + 4HCl(aq)$

   $NaOH(aq) + HCl(aq) \rightarrow NaCl(aq) + H_2O$

   or

   $Ca(OH)_2(aq) + 2HCl(aq) \rightarrow CaCl_2(aq) + 2H_2O$

3a. **Waste Treatment (50 MT/yr unit)**

   $Cl_2(g) + 2NaOH(aq) \rightarrow NaOCl(aq) + NaCl(aq) + H_2O$

Table 3.5-4

Raw Material Requirements for BCL Process (Case B)

Raw Material	Requirements lb/KG of Silicon
1. Silicon Tetrachloride, $SiCl_4$	15.33
2. Zinc, Zn	0.54
3. Caustic (50%), NaOH(aq)	3.75
or	
Lime (99%), $Ca(OH)_2$	1.75
4. Argon	3.1 SCF*
5. Nitrogen	7.6 SCF*
6. Chlorine, Cl_2 (by-product)	11.12

*Estimate from BCL

TABLE 3.5-5 UTILITY REQUIREMENTS FOR BCL PROCESS (Case B)

Utility/Function		Requirements/Kg of Silicon Product
1. Electricity		29.40 Kw-hr
1. Low Voltage D.C. for Electrolysis	(20.51)	
2. Zinc Vaporizer Induction Heated	(4.37)	
3. Preheat Section of Deposition Unit Induction Heated	(1.12)	
4. Electrolysis Feed Tank Heater	(0.24)	
5. Molten Zinc Storage Heater	(0.10)	
6. $SiCl_4$ Vaporizer	(0.53)	
7. Pumps, Blowers	([illegible].53)	
2. Steam (50 PSIA)		9.67 pounds
1. #1 Purification Column Calandria	(4.59)	
2. #2 Purification Column Calandria	(4.30)	
3. Caustic Storage Heating	(0.29)	
4. #1 Purification Column Preheater	(0.49)	
3. Cooling Water		34.49 Gallons
1. #1 Purification Column Condenser	(16.94)	
2. #2 Purification Column Condenser	(15.88)	
3. Purified Tet Cooler	(1.67)	
4. Process Water		10.48 Gallons
1. Diluent for Waste Treatment	(10.48)	
5. Refrigeration		2.38 MBtu
1. Reactor $SiCl_4$ Condenser (H-11)	(1.28)	
2. $SiCl_4$ Vent Condenser (H-07)	(1.10)	

TABLE 3.5-6

LIST OF MAJOR PROCESS EQUIPMENT FOR BCL (Case B)

	Equipment	Function	Size/Type	Material of Construction	Capacity Ratio to 1000 MT/yr
PROCESS TOWER AND INTERNALS					
1.	D-01 Light End Distillation Column	To purify $SiCl_4$	8" dia. x 21', packed 13.5'	Column, CS/packing, SS	20
2.	D-02 Heavy End Distillation Column	To purify $SiCl_4$	8" dia. x 21', packed 13.5'	Column, CS/packing, SS	20
3.	A-01 Primary $SiCl_4$ Vent Scrubber	To scrub $SiCl_4$ vent gas	3' dia. x 4'4" T/T, 225 gal/flat bottom	FRP	1
4.	A-02 Final $SiCl_4$ Vent Scrubber	To scrub $SiCl_4$ vent gas	7'6" dia. x 17'4" T/T/ 4 pp trays, Teflon dimister	FRP	1
HEAT EXCHANGER					
5.	H-01 L.E. Column Feed Heater	To preheat feed to D-01	2' dia. x 5', 15,013 Btu/hr / external heater	CS	20
6.	H-02 L.E. Column Reboiler	Reboiler of D-01	2' dia. x 3', 51,522 Btu/hr / external heater	CS	20
7.	H-03 L.E. Column Condenser	Total condenser of D-01	47,430 Btu/hr/shell-tube H.E.	CS	20
8.	H-04 H.E. Column Feed Heater	To preheat feed to D-02	2' dia. x 5', 14,331 Btu/hr/external heater	CS	20

TABLE 3.5-6 (Continued)

9.	H-05 H.E. Column Reboiler	Reboiler of D-02	2' dia. x 3', 56,641 Btu/hr/external heater	CS	20
10.	H-06 H.E. Column Condenser	Total condenser of D-02	52,292 Btu/hr/shell-tube H.E.	CS	20
11.	H-07 $SiCl_4$ Vent Condenser	Condense $SiCl_4$ from vent gas	38 ft^2, 18,000 Btu/hr/shell-tube H.E.	CS	20
12.	H-08 $SiCl_4$ Vaporizer	To provide $SiCl_4$ vapor to reactor	2.75' dia. x 3' T/T, 13,648 Btu/hr/resistance heater	CS	40
13.	H-09 Reactor Condenser	To condense by products from reactor	14" dia. x 6.4', 126,237.2 Btu/hr	Graphite W/SS shell	40
14.	H-10 Reactor $ZnCl_2$ Stripper	To condense $ZnCl_2$ gas	12 ft^2, 2,652 Btu/hr/shell-tube H.E., finned U-tube	316 SS	20
15.	H-11 $SiCl_4$ Condenser	To condense $SiCl_4$ gas for recycle	6,401 Btu/hr (x 4.62 = 29.573 Btu/hr)	316 SS	20
16.	H-12 Cell $ZnCl_2$ Stripper	To condense $ZnCl_2$ vapor	9,841.4 Btu/hr/shell-tube, H.E. (x 0.32)	Inconel 600	20
17.	H-13 Therminol Cooler (cold circuit)	To cool Therminol 66	68 ft^2, 11,000 Btu/hr/shell-tube H.E., 500 psia	CS	20
18.	H-14 Therminol Cooler (hot circuit)	To cool Therminol 66	262 ft^2, 120,000 Btu/hr/shell-tube H.E., 500 psia	CS	20
19.	H-15 Start-up Heater	Therminol start-up heater	98,950 Btu/hr/U-tube 15', resistance heater	CS	20
20.	H-16 Silicon Product Cooler (two)	To cool the Si product from reactor	5,735 Btu/hr	SiC	40

TABLE 3.5-6 (Continued)

20a.	H-17 Chlorination Cooler		20,000 Btu/hr, Area 200 ft^2	SS	1
20b.	H-18 Cell Gas Cooler		1.08×10^5 Btu/hr, Area 1805 ft^2	CS	1
	PROCESS AND STORAGE VESSELS				
21.	T-01 $SiCl_4$ Storage Tank	Storage/feed to purification	7' dia. x 16' T/T/ 4,600 gal	CS	20
22.	T-02 $SiCl_4$ Emergency Storage Tank	Storage/feed to purification	7' dia. x 16' T/T/ 4,600 gal	CS	20
23.	T-03 L.E. Column Reflux Drum	To hold distillate for reflux	12" dia. x 4'/23 gal	CS	20
24.	T-04 Surge Tank	Surge Tank for D-01 bottom	3' dia. x 4'/200 gal	CS	20
25.	T-05 Sump Tank	Sump for purification unit	3' dia. x 4'/200 gal	CS	20
26.	T-06 H.E. Column Reflux Drum	To hold distillate for reflux	12" dia. x 4'/23 gal	CS	20
27.	T-07 Pure $SiCl_4$ Storage Tank	Storage/feed to $SiCl_4$ Vaporizer	6' dia. x 10' T/T/ 1900 gal	CS	20
28.	T-08 Electrolysis Feed Tank	Storage/feed $ZnCl_2$ to electrolysis cell	50" x 158" x 38"H/ 7" graphite TH	Graphite/304 SS	20
29.	T-09 Molten Zinc Storage Tank	Storage/feed to Zinc vaporizer	W/heater 68,242 Btu/hr	Graphite/304 SS	20
30.	T-10 Therminol Head Tank	Storage Therminol	1.5' dia. x 3.75' T/T/ 43.6 gal	CS	20

TABLE 3.5-6 (Continued)

31.	T-11 Therminol Drain Down Tank	To store drained Therminol	2.75' dia. x 3' T/T/ 133 gal	CS	20
32.	T-12 Chlorine Supply Tank	To supply chlorine gas	1 1/2' dia. x 3'/ 37.62 gal	CS	20
33.	T-13 Lime Storage Tank	Storage Lime	12' dia. x 14'6" T/T/ 12,000 gal	FRP	1
PUMPS WITH DRIVERS					
34.	P-01 Purification Feed Pump	To feed $SiCl_4$ to storage tank	30 gpm, 31' head/ centrifugal, 1 1/2 hp	CS	20
35.	P-02 L.E. Column Feed Pump	To supply $SiCl_4$ to preheater	28.9 gph, Δp = 72 psia/ 0.5 hp.	CS	20
36.	P-03 L.E. Column Relux Pump	D-01 Reflux	51.7 gph, Δp = 23 psia/ 0.5 hp.	CS	20
37.	P-04 Surge Tank Pump	To supply $SiCl_4$ to H.E. Column	29.4 gph, Δp = 53 psia/ 0.5 hp.	CS	20
38.	P-05 Sump Pump	To pump $Sicl_4$ to emergency tank	30 gpm, 31' head/ centrifugal, 1 1/2 hp.	CS	20
39.	P-06 L.E. Column Bottom Pump	To pump $SiCl_4$ to surge tank	29.4 gph, Δp = 53 psia/ 0.5 hp.	CS	20
40.	P-07 H.E. Column Relux Pump	D-02 Reflux	57.1 gph, Δp = 25 psia/ 0.5 hp.	CS	20
41.	P-08 H.E. Column Bottom Pump	To pump bottom solution to waste treatment	1.3 gph, Δp = 25 psia/ 0.5 hp.	CS	20
42.	P-09 $SiCl_4$ Vaporizer Feed Pump	To feed $SiCl_4$ to Vaporizer	15 gph, 31' head/ 1/2 hp	CS	20

TABLE 3.5-6 (Continued)

43.	P-10 Reactor Condenser Circulating Pump	To circulate condensates	2.4 gpm, 30' head/1/2 hp	Graphite	40
44.	P-11 Cold Circuit Pump (two)	Cold Therminol circulation	20 gpm, 85' head/centrifugal, 2 hp.	CS	20
45.	P-12 Hot Circuit Pump	Hot Therminol circulation	62 gpm, 85' head/centrifugal, 4 hp.	CS	20
46.	P-13 Primary Scrubber Recirculation Pump	Recirculation for Scrubber A-01	20 gpm, 125' head/ centrigugal, 2.5 hp.	Duriron	1
47.	P-14 Primary Scrubber Lower-loop Recirculating Pump	Circulate solution for Lower-loop of Scrubber A-02	100 gpm, 103' head/ centrifugal, 7 1/2 hp.	Duriron	1
48.	P-15 Primary Scrubber Upper-loop Recirculating Pump	Circulate solution for upper-loop of Scrubber A-02	100 gpm, 13' head/ centrifugal, 2 hp.	Duriron	1
49.	P-16 Make up Lime Metering Pump	Lime make up	0.9 gpm, 25' head/ centrifugal, 1/2 hp.	CS	1

FILTERS

50.	F-01 L.E. Column Feed Filter	Remove solids	29 gph, Δp = 5 psia/ 140 micron	CS	20
51.	F-02 L.E. Column Reflux Filter	Remove solids	30 gph, Δp = 5 psia/ 140 micron	CS	20
52.	F-03 H. E. Column Feed Filter	Remove solids	52 gph, Δp = 5 psia/ 140 micron	CS	20
53.	F-04 H.E. Column Relfux Filter	Remove solids	31 gph, Δp = 5 psia/ 140 micron	CS	20

TABLE 3.5-6(Continued)

54.	F-05 Therminol Cooler Blower Filter	To filter the solids from air			20

SPECIALIZED EQUIPMENTS

55.	R-01 Fluidized Bed Reactor (two)	To reduce $SiCl_4$ to Si by Zn	1830.2 Btu/hr, 6.5" dia.	Graphite Lined / SS	40
56.	FN-01 Furnace (two)	To preheat $SiCl_4$ gas	272,966 Btu/hr		40
57.	B-01 Seed Addition Hopper (two)	To feed Si seed to the reactor		310 SS	40
58.	B-02 Si Product Hopper (four)	To hold Si product	6 gal	310 SS	20
59.	B-03 Zinc Hopper	To hold make up Zinc	40 gal	CS	20
60.	C-01 Therminol Cooler Blower	Therminol system air cooler blower	500 acfm fan/electric, 1 1/2 hp., 12-1/2" wheel	CS	20
61.	C-02 Scrubber Vent Blower	Suck $SiCl_4$ gas for A-01 & A-02	10,000 acfm/electric, 50 hp. 31-1/2" wheel	FRP	1
62.	E-01 Eductor (two)	$SiCl_4$ scrubbing (Scrubber D-05)	20 gpm, Δp = 47.4 psia/ Hydraulic ejector, 1-1/2" NPT	P.V.C.	1
63.	EC-01 Electrolysis Cell (six)	To recover Zn from $ZnCl_2$	5,000 ~6,000 amp cells	Graphite/SS	60
64.	PW-01 Power Supply	To supply power to electrolysis cell	545,933 Btu/hr.		20
65.	VP-01 Zinc Vaporizer (two)	To provide zinc vapor to reactor	104,128.8 Btu/hr 13.5" dia. x 32"	Quartz	40

TABLE 3.5-6 (Continued)

NOTE:

1. For the 1000 MT/yr plant, items 3, 4, 33, 46, 47, 48, 49, 61, and 62 are used for waste treatment of distillation wastes (light, heavy) and vent gases.
2. In the 50 MT/yr facility, these items are used for hypochlorite maufacture which is not present in the 1000 MT/yr plant.
3. For E-11, the operation conditions were changed from 171°F - 32°F to 662°F - 20°F.
4 For E-12, the operation conditions have been chnaged from T = 855°F to 270°F.

TABLE 3.5-7

PRODUCTION LABOR REQUIREMENTS FOR BCL PROCESS (Case B)

Section		Labor man-hr/KG Si (oper/shift)
1. Purification	(I)	0.01402 (2)
2. Deposition	(II)	0.01402 (2)
3. Electrolysis	(III)	0.02103 (3)
4. Waste Treatment	(IV)	0.00701 (1)
5. Product Handling	(V)	0.00701 (1)
	TOTAL	0 06309 (9)

Note

Manpower estimate for production labor requirements based on:

1. Dividing plant into sections
   -type of unit operation
   -mark off working area
2. Specify work duties required in each section
3. Estimate operators required to perform work duties in each section
   -type of unit operation
   -size of working area
   -degree of automation (batch, semi-continuous, continuous, etc.)

3.6 DCS Process (Dichlorosilane)

The chemical engineering analysis activity involves a preliminary process design of a palnt to produce dichlorosilane as a silicon source material by using the technology under consideration.

The process flowsheet for the DCS process to produce dichlorosilane consisting several major processing operations of hydrochlorination, condensation, stripping, distillation and redistribution reaction, is shown in Figure 3.6-1.

Metallurgical grade silicon (M.G.Si) is hydrochlorinated at the presence of hydrogen (H_2) and silicon tetrachloride ($SiCl_4$) in a fluidized bed reactor.[2] The product stream from the hydrochlorination is cooled, A settler is then used to remove metal impurities. The chlorosilanes - dichlorosilane (DCS), trichlorosilane (TCS) and silicon tetrachloride (TET) are separated by several distillation units. After separation, the silicon tetrachloride is recycled.

Intermediate in the several distillation units, the TCS is redistributed to DCS and TET by passing through a fixed bed of catalyst. After redistribution the stream is fed to appropriate distillation unit for separation and purification. The reaction equations to produce DCS are shown

$$3SiCl_4 + Si + 2H_2 \rightarrow 4SiHCl_3 \qquad (3.6\text{-}1)$$

$$2SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4 \qquad (3.6\text{-}2)$$

A process design was performed to obtain data for a cost analysis of a plant to produce DCS by this new technology. The design was based on a palnt to produce 3,780 metric tons/yr of DCS which is sufficient to produce 1000 metric tons/yr of silicon without recycle.

The detailed status sheet for the process design package is shown in Table 3.6-1 and is representative of the various subitems that make up the activity. 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:

- Base Case Conditions . . . Table 3.6-2
- Reaction Chemistry . . . Table 3.6-3
- Raw Material Requirements . . . Table 3.6-4
- Utility Requirements . . . Table 3.6-5
- Major Process Equipment . . . Table 3.6-6
- Production Labor Requirements . . . Table 3.6-7

The process design provides detailed data for raw materials, utilities, major process equipment and production labor requirements which are necessary for polysilicon production.

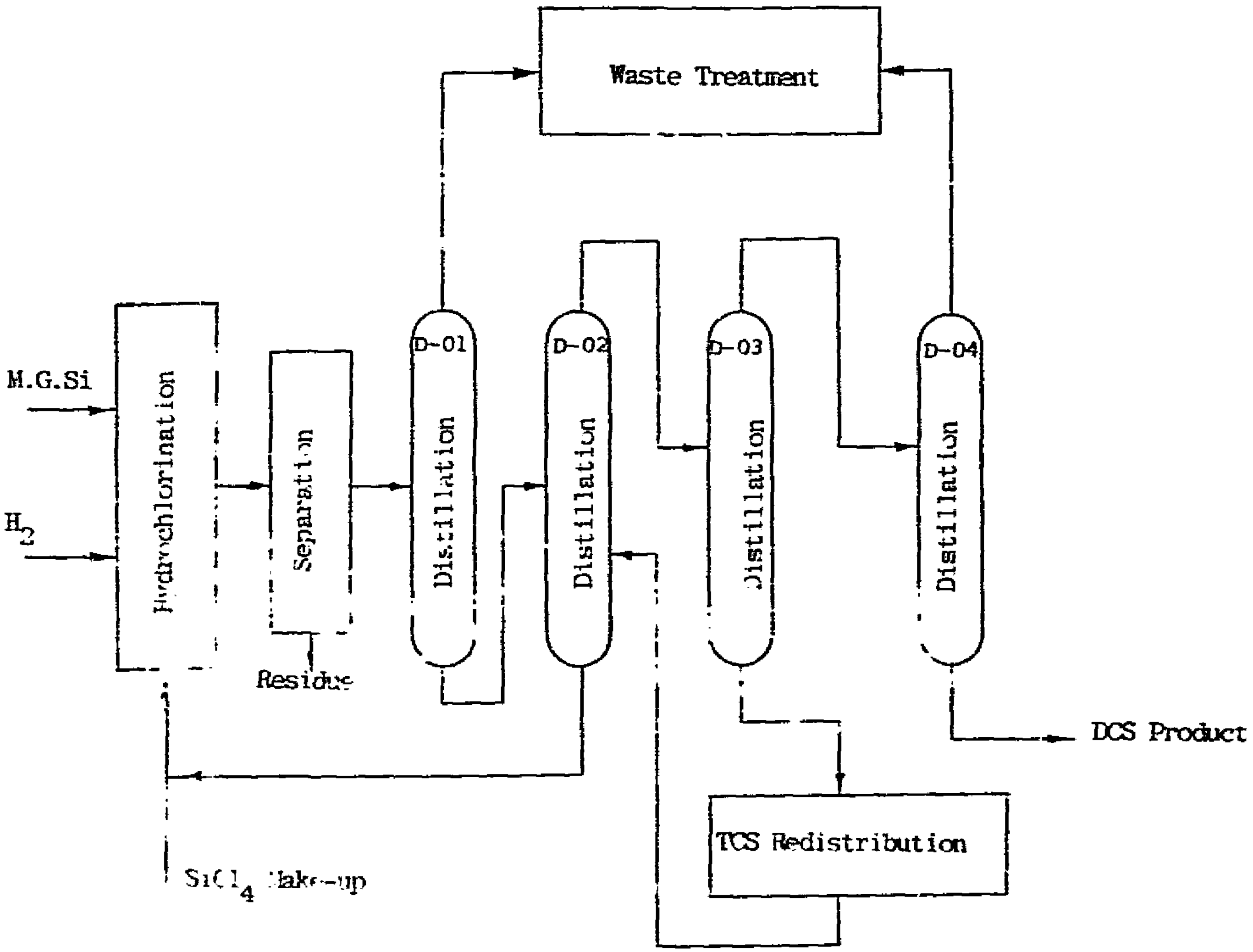


Figure 3.6-1 Process Flowsheet for DCS Process

TABLE 3.6-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR DCS PROCESS

Prel. Process Design Activity	Status
1. Specify Base Case Conditions	●
1. Plant Size	●
2. Product Specifics	●
3. Additional Conditions	●
2. Define Reaction Chemistry	●
1. Reactants, Products	●
2. Equilibrium	●
3. Process Flow Diagram	●
1. Flow Sequence, Unit Operations	●
2. Process Conditions (T, P, etc.)	●
3. Environmental	●
4. Company Interaction (Technology Exchange)	●
4. Material Balance Calculations	●
1. Raw Materials	●
2. Products	●
3. By-Products	●
5. Energy Balance Calculations	●
1. Heating	●
2. Cooling	●
3. Additional	●
6. Property Data	●
1. Physical	●
2. Thermodynamic	●
3. Additional	●

Prel. Process Design Activity	Status
7. Equipment Design Calculations	●
1. Storage Vessels	●
2. Unit Operations Equipment	●
3. Process Data (P, T, rate, etc.)	●
4. Additional	●
8. List of Major Process Equipment	●
1. Size	●
2. Type	●
3. Materials of Construction	●
8a. Major Technical Factors	●
(Potential Problem Areas)	●
1. Materials Compatibility	●
2. Process Conditions Limitations	●
3. Additional	●
9. Production Labor Requirements	●
1. Process Technology	●
2. Production Volume	●
10. Forward for Economic Analysis	●

0 Plan
◐ In Progress
● Complete

TABLE 3.6-2

BASE CASE CONDITIONS FOR DCS PROCESS

1. Plant Size
   - Dichlorosilane produced from m.g. silicon and silicon tetrachloride.
   - 2,895 lb/hr dichlorosilane (enough to support 1000 metric tons/year of silicon production)
   - 9,780 metric tons/yr of DCS capacity

2. Hydrochlorination
   - Metallurgical grade silicon, hydrogen, and recycle silicon tetrachloride (TET) used to produce trichlorosilane (TCS)
   - Copper catalyzed
   - Fluidized bed
   - 500°C, 514.7 psia
   - H_2/Cl_2 ration about 2.8
   - 30% conversion of $SiCl_4$ to $SiHCl_3$

3. TCS Redistribution Reaction
   - TCS is redistributed to DCS and TET through catalytic reaction
   - Catalytic redistribution of TCS with amine function ion exchange resin
   - Liquid phase 85 psia, 140°F
   - Conversion from pure TCS feed is about 11% to DCS

4. Recycles
   - Unreacted chlorosilanes and hydrogen are separated by distillation and recycled

5. Dichlorosilane Purification
   - Final purification by distillation
   - Designed to remove trace impurities (B_2H_6, example)

6. Operating Ration
   - Approximately 85% utilization (on stream time)
   - Approximately 7446 hour/year production

7. Storage Consideration
   - Feed materials (several week supply, approx. 1 month)
   - Product (two shifts storage)
   - Process (several hours to 1 shift)

TABLE 3.6-3

REACTION CHEMISTRY FOR DCS PROCESS

1. Hydrochlorination Reaction

$$3SiCl_4 + Si + 2H_2 \rightleftarrows 4SiHCl_3$$

2. Redistribution Reaction

$$2SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4$$

3. Waste Treatment (representative - overall)

$$SiH_2Cl_2 + Ca(OH)_2 \xrightarrow{aq.} SiO_2 + CaCl_2 + 2H_2O$$

$$SiHCl_3 + 1.5Ca(OH)_2 \xrightarrow{aq.} SiO_2 + 1.5CaCl_2 + 2H_2O$$

$$SiCl_4 + 2Ca(OH)_2 \xrightarrow{aq.} SiO_2 + 2CaCl_2 + 2H_2O$$

Note:

1. Reaction 1 product contains H_2, HCl, $SiCl_4$, $SiHCl_3$, SiH_2Cl_2 (trace), other trace chlorides

2. Reaction 2 product contains $SiCl_3$, $SiCl_4$, SiH_2Cl_2, SiH_3Cl

TABLE 3.6-4

RAW MATERIAL REQUIREMENTS FOR DCS PROCESS

	Raw Material	Requirements lb/hr	lb/kg of DCS
1.	M.G. Silicon (Si)	456.6	0.348
2.	Silicon Tetrachloride ($SiCl_4$, make-up)	2609.5	1.987
3.	Liquid Hydrogen	62.5	0.048
4.	Copper Catalyst (Cu)	6.8	0.005
5.	Hydrate Lime ($Ca(OH)_2$)	310.0	0.236

TABLE 3.6-5

UTILITY REQUIREMENTS FOR DCS PROCESS

Utilities/Function	Total Requirements	Requirements per Kg of DCS
1. Electricity		
1) Gas Compressions (96bhp)	217 KW	.165 KW-Hr
2) Pumping Liquids (98.5 bhp)	223 KW	.170 KW-Hr
3) Filter Drive (1 bhp)	2.3 KW	.002 KW-Hr
	443 KW	.337 KW-Hr
2. Steam (50 psia, saturated)		
1) Column Reboiler (12.0MM Btu/hr)	3,850 lb/hr	2.93 lb
2) Vaporizer (3.56MM Btu/hr)	12,970 lb/hr	9.88 lb
	16,820 lb/hr	12.81 lb
3. Cooling Water		
1) Coolers and Condensers (21.66MM Btu/hr)	1237 gpm	56.51 gal
4. Process Water		
1) Waste Treatment	6.59 gpm	.301 gal
5. Fuel Oil		
1) Direct-Fired Heater (4.71MM Btu/hr)	33.4 gal/hr	.026 gal
2) Incineration (1.5×10^6MM Btu/hr)	10.6 gal/hr	.008 gal
	44.0 gal/hr	.034 gal

TABLE 3.6-6

LIST OF MAJOR PROCESS EQUIPMENT FOR DCS PROCESS

	Equipment	Function	Duty/Type	Size	Material of Construction
	Reactors				
1.	R-01 Hydrochlorination Reactor	Hydrochlorination of m.g. Si & $SiCl_4$	32,200lb/hr Feed/Fluid. bed	8.54' diam. x 9.75', and 12.25', 30° cone	316SS
2.	R-02 TCS Redistribution Reactor	Conversion of TCS to DCS	31,000lb/hr Feed/Fixed Bed, catalyst	2' diam. x 36' 320 psia	316SS
3.	R-03 Waste Neutralizer	Waste Treatment	agitated vessel	3' diam. x 20' 14.7 psia	316SS
4.	R-04 Waste Combuster	To incinerate waste vapors	25 SCFM Vapor/Combustion	3' x 3' x 9' 14.7 psia	CS/Brick
	Distillation Columns				
5.	D-01 Crude TCS Stripping Column	To remove inert gases	31,217lb/hr of feed	24" diam. x 20' tall with 10 sieve plates	CS
6.	D-02 TCS/STC Distillation Column	To remove STC at bottom	62,208.4lb/hr of feed	5.2' diam. x 68'tall with 29 sieve plates	CS
7.	D-03 DCS/TCS Distillation Column	To remove DCS at distillates	34,001.2lb/hr of feed	4.9' diam. x 102'tall with 46 sieve plates	CS
8.	D-04 DCS Distillation Column	To purify DCS	3,009.8lb/hr of feed	1.1' diam. x 70' tall with 40 sieve plates	316SS

TABLE 3.6-6 (continued)

	Equipment	Function	Duty/Type	Size	Material of Construction
	Tanks & Bins				
9.	B-01 Silicon Storage Bin with Feed Lock	To store and feed m.g. Si to reactor	1 week storage/Vertical, with Feed Lock	7'diam. x 22', 60°cone	CS
10.	T-01 Residue Setting Tank	To separate unreacted solid residues	Vertical	8' diam. x 16', 515 psia	316SS
11.	T-02 Residue Withdraw Tank	To remove unreacted solid residues	Vertical	3' diam. x 6', 515 psia	316SS
12.	T-03 Hydrogen Separation Tank	To separate H_2 gas from chlorosilanes	Vertical, mesh pad	3.75' diam. x 11.25', 515 psia	CS
13.	T-04 Crude TCS Storage Tank	To store crude TCS	8 hr. storage, Horizontal	12'diam. x 33', 100 psia	CS
14.	T-05 TCS Stripper Reflux Drum	Reflux drum for D-01 column	30 min. storage, Vertical	2' diam. x 3.5', 90 psia	CS
15.	T-06 TCS/STC Distillation Reflux Drum	Reflux drum for D-02 column	10 min. storage, Vertical	4.5' diam. x 19', 55 psia	CS
16.	T-07 STC Storage Tank	To store STC	6 hr. storage, Horizontal	10.25' diam. x 3.05', 15 psia	CS
17.	T-08 DCS/TCS Distillation Reflux Drum	Reflux drum for D-03 column	10 min. storage, Vertical	4' diam. x 13', 320 psia	CS
18.	T-09 DCS Distillation Reflux Drum	Reflux drum for D-04 column	10 min. storage, Vertical	1.5' diam. x 4.25', 125 psia	316SS
19.	T-10 DCS Storage Tank	To store purified DCS	8 hr. storage, Horizontal	6' diam. x 16.75', 125 psia	316SS

TABLE 3.6-6 (continued)

	Equipment	Function	Duty/Type	Size	Material Construction
20.	T-11 Flue Gas Separation Tank	To separate flue gas from lime solution	Vertical tank with mesh	2' diam. x 5'	CS
21.	T-12 Lime Solution Preparation Tank	To prepare lime solution	8 hr. storage, Vertical, open top	5' diam. x 9.5'	CS
22.	T-13 Waste Filtrate Storage Tank	To store waste filtrate	4 hr. storage, vertical	5' diam. x 8'	CS
	Heaters & Heat Exchangers				
23.	H-01 Crude TCS Condenser	To condense chlorosilanes	8.4MM Btu/Hr. Shell-Tube H.E.	1211 ft^2, 515 psia	316SS
24.	H-02 H$_2$ Gas Preheater	To preheat H$_2$ Gas for chlorination	500°C discharge, Direct-fired heater	2.59MM Btu/hr, 515 psia	CS/316SS
25.	H-03 STC Vaporizer	To vaporize and superheat STC for chlorination	3.56MM Btu/hr, Kettle	573 ft^2, 515 psia	316SS
26.	H-04 Stripper Condenser	Partial condenser for D-01 column	86,700 Btu/hr Shell-tube H.E.	30 ft^2, 90 psia	CS
27.	H-05 Stripper Reboiler	Stripper reboiler of D-01 column	0.91MM Btu/hr, Kettle	40 ft^2, 95 psia	CS
28.	H-06 TCS Condenser	To condense TCS vapor of D-02 column	7.9MM Btu/hr, Shell-tube H.E.	2,358 ft^2, 55 psia	316SS
29.	H-07 TCS/STC Reboiler	Reboiler for D-02 TCS/STC Distillation column	8.25MM Btu/hr, Kettle	318 ft^2, 55 psia	CS
30.	H-08 STC Heat Exchanger	STC Cooling and Heating	0.824MM Btu/hr, Liq-liq. heat exchanger	742 ft^2, 55 psia	316SS/CS

TABLE 3.6-6 (continued)

	Equipment	Function	Duty/Type	Size	Material of Construction
31.	H-09 DCS Condenser	To condense DCS Vapor from D-03 Column	3.2MM Btu/hr Shell-Tube H.E.	328 ft^2, 320 psia	316SS/CS
32.	H-10 DCS/TCS Reboiler	Reboiler for DCS/TCS distillation column, D-03	2.7MM Btu/hr, Kettle	252 ft^2, 320 psia	CS
33.	H-11 TCS Cooler	To cool TCS before redistribution reaction	1.32MM Btu/hr Shell-Tube H.E.	78.6 ft^2, 85 psia	316SS
34.	H-12 DCS Distillation overhead condenser	To condense overhead of D-04 column	0.183MM Btu/hr Shell-Tube H.E.	23.4 ft^2, 355 psia	316SS/CS
35.	H-13 DCS Distillation Reboiler	Reboiler of DCS Distillation column,D-04	0.12MM Btu/hr	6.8 ft^2, 355 psia	316SS/CS
36.	H-14 Waste stream cooler	To cool waste stream in waste treatment	0.5MM Btu/hr Shell-Tube H.E.	125 ft^2, 60 psia	316SS/CS
37.	H-15 STC Superheater	To heat STC before hydrochlorination	500°C discharge temp. Direct-fired heater	2.12MM Btu/hr, 515 psia	316SS/CS
38.	H-16 H_2 Compressor Intercooler	To cool H_2 gas between compression stages	70,000 Btu/hr Shell-Tube H.E.	67.7 ft^2, 90 psia	316SS/CS
	Compressors and Pumps				
39.	C-01A Hydrogen Feed Compressor. First stage	Compression of recycle and make-up H_2 gas	187 SCFM/Recip.comp.	38bhp. discharge press. 87 psia	CS
40.	C-01B Hydrogen Feed compressor, Second stage	Compression of recycle and make-up H_2 gas	187 SCFM/Recip.comp.	41bhp., discharge press. 515 psia	CS

TABLE 3.6-6 (continued)

	Equipment	Function	Duty/Type	Size	Material of Construction
41.	C-02 Hydrogen Circulation Compressor	Compression of recycle H_2 gas	2,833 SCFM/centri-	17bhp., ΔP=30 psi	CS
42.	P-01 Feed Tank Blower	To load silicon to its storage bin	Pnumatic transport/ centrifugal blower	939ACFM, 32bhp	CS
43.	P-02 Settling Tank Circulation Pump	Circulation and to support ejector	100 gpm centrifugal	37' Head, 1.75bhp	316SS
44.	P-04 TCS Reflux Pump	Pumping TCS for D-02 reflux and feed to D-03	58 gpm centrifugal	12bhp, discharge press. 320 psia	CS
45.	P-05 STC Feed Pump	Pumping STC to Hydrochlorination reactor	42.2 gpm centrifugal	15bhp, discharge press. 500 psia	CS
46.	P-06 DCS Reflux Pump	Pumping DCS for D-03 reflux and feed to D-04	6.5 gpm centrifugal	¼bhp, discharge press. 355 psia	316SS
47.	P-08 DCS Purification Discharge Pump	To withdraw impurities from DCS Purification unit	2.6 gpm centrifugal	¼ bhp, discharge press. 355 psia	316SS
48.	P-09 DCS Pump	To pump pure DCS	290 gpm centrifugal	34 bhp	316SS
49.	P-10 Waste Solution Pump	To feed slurry to filter	12.5 gpm centrifugal	1.25 bhp	Cast Iron
50.	P-11 Lime Solution Circulation Pump	To circulate lime solution to neutralizer	12.5 gpm centrifugal	1.25 bhp	Cast Iron
51.	P-12 Fresh Lime Solution Pump	To supply fresh lime solution	6.5 gpm centrifugal	0.75 bhp	Cast Iron

TABLE 3.6-6 (continued)

	Equipment	Function	Duty/Type	Size	Material of Construction
	Miscellaneous				
52.	F-01 Silicon Dust Filter	To retain m.g. silicon dust	Gas-Solid/Bag	20 ft^2 x 5μ	CS/cloth
53.	F-02 Waste Slurry Filter	To remove waste sludge	12.5 gpm rotary filter	2 ft^2	CS/cloth
54.	S-01 Silicon Feed Cyclone	To feed m.g. silicon to storage bin	6" w.c.ΔP	940ACFM	316SS
55.	E-01 Quench Contact Ejector	To withdraw and cool effluent of hydrochlorination	6" w.c. suction	100 gpm 134 ACFM	316SS
56.	E-02 Flue Gas Ejector	To withdraw flue gas from waste gas combustion	10" w.c. suction	100 gpm 1 SCFM	CS

TABLE 3.6-7

PRODUCTION LABOR REQUIREMENTS FOR DCS PROCESS

	Section	Labor man-hr/KG DCS	 (oper/shift)
1.	Hydrochlorination	0.001294	(2)
2.	Purification/Redistribution	0.00194	(3)
3.	Waste Treatment	0.000647	(1)
	TOTAL	0.003882	(6)

Note

Manpower estimate for production labor requirements based on

1. Dividing plant into sections
   - -type of unit operation
   - -mark off working area
2. Specify work duties required in each section
3. Estimate operators required to perform owrk duties in each section
   - -type of unit operation
   - -size of working area
   - -degree of automation (batch, semi-continuous, etc.)

4. ECONOMIC ANALYSES

4.1 SiI_4 Decomposition Process

The economic analysis activity involves a cost analysis of the process under consideration for the production of silicon. The cost analysis for the particular technology is based on process design results, such as requirements for raw materials and major process equipment necessary to produce the product, from the chemical engineering analysis activity. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silicon by the SiI_4 decomposition process are presented in Table 4.1-1 including costs for raw materials, labor utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of $44.64 (1975 dollars) and $62.50 (1980 dollars) per kg. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses.

The product cost represents all cost associated with producing silicon. On top of these costs a producing company will includes some profit. The sales price of the product silicon will actually be the sum of the product cost and a profit for the company. The profit is usually measured in terms of rate of return on the capital investment that the company spent in going into the polysilicon business. Two profitability methods which are commonly used are the return on original investment (per cent ROI) and discounted cash flow rate of return (per cent DCF).

The cost and profitability analysis summary for this process are presented in Table 4.1-2. The sales price of polysilicon at various rates of return for both profitability methods (per cent ROI and DCF) is shown in the lower half of the table. The results indicate a sales price of $71.48 per kg of silicon (1980 dollars) at 5 per cent DCF return on investment.

These cost and profitability results for the SiI_4 decomposition process indicate that this new technology for producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities..Table 4.1-3
- Process Design Inputs....................Table 4.1-4
- Base Case Conditions......................Table 4.1-5
- Raw Material Cost.........................Table 4.1-6
- Utility Cost..............................Table 4.1-7
- Major Process Equipment Cost..............Table 4.1-8
- Production Labor Cost.....................Table 4.1-9
- Plant Investment..........................Table 4.1-10
- Total Product Cost........................Table 4.1-11

TABLE 4.1-1

ESTIMATION OF PRODUCT COST FOR SiI_4 DECOMPOSITION PROCESS

		Cost $/Kg of Silicon (1975 dollars)	Cost $/Kg of Silicon (1980 dollars)
1.	Direct Manufacturing Cost (Direct Costs)	23.48	32.87
	Raw Materials		
	Direct Operating Labor		
	Utilities		
	Supervision and Clerical		
	Maintenance and Repairs		
	Operating Supplies		
	Laboratory Charge		
2.	Indirect Manufactuing Cost (Fixed Cost)	12.17	17.04
	Depreciation		
	Local Taxes		
	Insurance		
3.	Plant Overhead	3.17	4.44
4.	General Expenses	5.82	8.15
	Administration		
	Distribution and Sales		
	Research and Development		
5.	Product Cost Without Profit	44.64	62.50

TABLE 4.1-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR SiI_4 DECOMPOSITION PROCESS

1. Process....................................SiI_4 Decomposition Process
2. Plant Size..................................1,000 Metric Tons/year
3. Plant Product...............................Silicon
4. Product Form................................Silicon Ingots (Rods)
5. Plant Investment............................$107,600,000/$150,650,000 (1975 dollars) (1980 dollars)

Fixed Capital		$ 93.57 Mega	$131.00 Mega
Working Capital		$ 14.03 Mega	$ 19.65 Mega
(15%)	Total	$107.60 Mega	$150.65 Mega
		(1975 dollars)	(1980 dollars)

6. Return on Original Investment, after taxes (%ROI)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% ROI..............	44.64	62.50
5% ROI..............	54.60	76.45
10% ROI..............	64.57	90.40
15% ROI..............	74.53	104.35
20% ROI..............	84.49	118.30
25% ROI..............	95.46	132.25
30% ROI.............	104.42	146.19
40% ROI.............	124.35	174.09

7. Discounted Cash Flow Rate of Return, after taxes (% DCF)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% DCF..............	44.64	62.50
5% DCF..............	51.05	71.40
10% DCF..............	58.11	81.36
15% DCF..............	65.74	92.04
20% DCF..............	73.84	103.38
25% DCF..............	82.34	115.28
30% DCF..............	91.16	127.63
40% DCF..............	109.50	153.31

Based on 10 year project life and 10 year straight line depreciation.

8. Tax Rate (Federal)..46%

TABLE 4.1-3

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR SiI_4 Decomposition Process

	Prel. Process Economic Activity	Status
1.	Process Design Inputs	●
	1. Raw Material Requirements	●
	2. Utility Requirements	●
	3. Equipment List	●
	4. Labor Requirements	●
2.	Specify Base Case Conditions	●
	1. Base Year for Costs	●
	2. Appropriate Indices for Costs	●
	3. Additional	●
3.	Raw Material Costs	●
	1. Base Cost/lb. of Material	●
	2. Material Cost/Kg of Silicon	●
	3. Total Cost/Kg of Silicon	●
4.	Utility Costs	●
	1. Base Cost for Each Utility	●
	2. Utility Cost/Kg of Silicon	●
	3. Total Cost/Kg of Silicon	●
5.	Major Process Equipment Costs	●
	1. Individual Equipment Cost	●
	2. Cost Index Adjustment	●

	Prel. Process Economic Activity	Status
6.	Production Labor Costs	●
	1. Base Cost Per Man Hour	●
	2. Cost/Kg Silicon Per Area	●
	3. Total Cost/Kg Silicon	●
7.	Estimation of Plant Investment	●
	1. Battery Limits Direct Costs	●
	2. Other Direct Costs	●
	3. Indirect Costs	●
	4. Contingency	●
	5. Total Plant Investment (Fixed Capital)	●
8.	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	●

○ Plan
◐ In Progress
● Complete

TABLE 4.1-4

PROCESS DESIGN INPUTS FOR
SiI_4 Decomposition Process

1. Raw Material Requirements
   - -Silicon tetrachloride, zinc, lime, argon and nitrogen
   - -see table for "Raw Material Cost"

2. Utility
   - -electricity, steam, cooling water and process water
   - -see table for "Utility Cost"

3. Equipment List
   - -41 plus pieces of major process equipment
   - -process vessels, heat exchangers, reactor, etc.

4. Labor Requirements
   - -production labor for purification, deposition, etc.
   - -see table for "Production Labor Cost"

TABLE 4.1-5
BASE CASE CONDITION FOR SiI_4 Decomposition 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

3. Raw Material Cost

   -Chemical Marketing Reporter
   -January 1975 Value
   -Raw Material Cost Index for Industrial Chemicals
   -1975 Cost Index Value = [illegible] (Wholesale Price Index, Producer Price Index)

4. Labor Cost

   -Average for Chemical Petroleum Coal and Allied Industries (1975)
   -Skilled $6.90/hr

5. Update to 1980

   -historically cited 1975 dollars (LSA project)
   -DOE decision to change to 1980 dollars (JPL, 6/22/79)
   -reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

TABLE 4.1-6

RAW MATERIAL COSTS FOR SiI_4 DECOMPOSITION PROCESS

	Raw Material	Requirement lb/Kg of Silicon	$/lb of Material	Cost $/Kg of Silicon
1.	Metallurgical Si	2.6194	.454	1.188
2.	Iodine*	.7495	2.59	1.94
3.	Iodine*	6.746	.20	1.35
			TOTAL COST	4.48

* SiI_4 wastes are recovered as iodine for recycle at $ .20/pound. Assuming 10% losses in this step, 10% of total iodine must be purchased at $2.59/pound.

TABLE 4.1-7

UTILITY COST FOR SiI_4 DECOMPOSITION PROCESS

Utility	Requirements in Kw-hr/ Kg of Silicon	Cost of Utility	Cost $/Kg of Silicon
Electricity*	218.62	$ .0324/Kw-hr	7.08

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* For costing purposes only. Actual utilities would involve cooling water, steam, etc.

TABLE 4.1-8

ESTIMATED COST OF MAJOR PROCESS EQUIPMENT FOR SiI_4 DECOMPOSITION PROCESS

	Equipment	Purchased Cost, $M
1.	Purified SiI_4 Hold Tank	63.80
2.	Liquid Reactor Overheads Storage	60.50
3.	Silicon Product Storage	6.72
4.	Liquid Iodine Storage	4.54
5.	SiI_4 Bulk Storage	67.19
6.	Metallurgical Silicon Storage	8.06
7.	Feed Tank for Purification Column 2	6.89
8.	SiI_4 Vaporizer	7.87
9.	Silicon Cooler	3.16
10.	Deposition Condenser	525.4
11.	Separation Column Preheater	3.48
12.	Separation Column O/H Condenser	15.45
13.	Separation Column Calandria	12.19
14.	Separation Column O/H After Cooler	3.09
15.	Iodine Vaporizer	7.86
16.	Iodination O/H Condenser	50.22
17.	Separation Column Bottoms After Cooler	3.48
18.	Tet Purification Preheater	7.73
19.	Tet Purification Column 1 O/H Condenser	15.45
20.	Tet Purification Column 1 Calandria	12.39
21.	Tet Purification Column 2 O/H Condenser	15.45
22.	Tet Purification Column 2 Calandria	12.06
23.	Tet Purification After Cooler	7.73

TABLE 4.1-8 (Continued)

	Equipment	Purchased Cost, $M
24.	Deposition De-superheaters (6 units)	38.68
25.	Purified SiI_4 Pump	1.76
26.	Deposition Compressor System	12090.0
27.	I_2/SiI_4 Liquid Pump	1.76
28.	I_2/SiI_4 Separation Column O/H Pump	1.76
29.	I_2/SiI_4 Separation Column Bottoms Pump	2.15
30.	Iodine Pump	2.15
31.	SiI_4 Pump	1.76
32.	Tet Purification Column 1 O/H Pump	1.76
33.	Tet Purification Column 1 Bottoms Pump	2.12
34.	Tet Purification Column 2 Feed Pump	1.25
35.	Tet Purification Column 2 O/H Pump	1.76
36.	Tet Purification Column 2 Bottoms Pump	2.09
37.	Deposition Units (6 units)	1922.0
38.	Iodination Reactor	10.75
39.	I_2/SiI_4 Distillation Column	16.50
40.	Tet Purification Column 1	47.25
41.	Tet Purification Column 2	24.44
	TOTAL PURCHASED COST	15090.65

TABLE 4.1-9

PRODUCTION LABOR COSTS
SiI_4 DECOMPOSITION PROCESS

	Skilled Man-Hrs/Kg Silicon	Semiskilled Man-Hrs/Kg Silicon	$Kg Si
1	.008395	-	.05793
2	.01314	-	.09067
3	.008395	-	.05793
4	.008395	-	.05793
5	.00584	-	.040296
6	.008395	-	.05793
7	.00584	-	.040296
8.	-	.01314	.064386
9.	-	.01314	.064386
			$ .5319/Kg

NOTES

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

TABLE 4.1-10

ESTIMATION OF PLANT INVESTMENT FOR SiI_4 DECOMPOSITION PROCESS

		Investment $1000
1.	DIRECT PLANT INVESTMENT COSTS	
	1. Major Process Equipment Cost	15,090.0
	2. Installation of Major Process Equipment	6,488.7
	3. Process Piping, Installed	11,166.6
	4. Instrumentation, Installed	2,867.1
	5. Electrical, Installed	1,509.0
	6. Process Buildings, Installed	1,509.0
1a.	SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	38,630.4
2.	OTHER DIRECT PLANT INVESTMENT COSTS	
	1. Utilities, Installed	7,243.2
	2. General Service, Site Development, Fire Protection, etc.	1,810.8
	3. General Buildings, Offices, Shops, etc.	2,112.6
	4. Receiving, Shipping Facilities	3,168.9
2a.	SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	14,335.5
3.	TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	52,965.9
4.	INDIRECT PLANT INVESTMENT COSTS	
	1. Engineering, Overhead, etc.	8,299.5
	2. Normal Cont. for Floods, Strikes, etc.	10,713.9
4a.	TOTAL INDIRECT PLANT INVESTMENT COST	19,013.4
5.	TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	71,979.3
6.	OVERALL CONTINGENCY, % of 5	21,593.8
7.	FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	93,573.1 (1975 dollars) x 1.4 inflation 131,002.3 (1980 dollars)

TABLE 4.1-11

ESTIMATION OF TOTAL PRODUCT COST FOR SiI_4 DECOMPOSITION PROCESS

	$/KG of Si	
1. Direct Manufacturing Cost (Direct Charges)		
1. Raw Materials	4.48	
2. Direct Operating Labor	.58	
3. Utilities	7.08	
4. Supervision and Clerical	.08	
5. Maintenance and Repairs	9.36	
6. Operating Supplies	1.87	
7. Laboratory Charge	.08	
2. Indirect Manaufacturing Cost (Fixed Charges)		
1. Depreciation	9.36	
2. Local Taxes	1.87	
3. Insurance	.94	
3. Plant Overhead	3.17	
4. By-Product Credit	-----	
4a. Total Manufacturing Cost, 1 + 2 + 3 + 4	38.82	
5. General Expenses		
1. Administration	2.33	
2. Distribution and Sales	2.33	
3. Research and Development	1.16	
6. Total Cost of Product, 4a + 5	44.64	(1975 dollars)
	x 1.4	inflation
	62.50	(1980 dollars)

4.2 Conventional Polysilicon Process (Siemen's Technology)

The economic analysis activity for the conventional polysilicon process involves a cost analysis for the production of silicon via the Siemen's technology. In the Siemen's technology, trichlorosilane (TCS) is used as the feed source material for semiconductor grade silicon.

Since several existing plants producing semiconductor grade polysilicon in the United States were constructed in the 1960's, the cost analysis is based on a poly plant constructed in the 1960's (1965 or earlier). Operating costs for the plant are applicable to the time period of interest (such as 1975 and 1980).

The cost analysis results for producing silicon by the conventional Siemen's process are presented in Table 4.2-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes these items to give a total product cost without profit of $35.52 - 41.29 (1975 dollars) and $49.73 - 57.81 (1980 dollars) per kg. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses. The range for product cost reflects low and high electrical costs (1.5-3¢/kw hr for 1975 and 2.1-4.2¢/kw hr for 1980).

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) for 1975 are considered representative based on a recent plant site survey listing industrial power cost in the USA. With respect to the intermediate value, the survey indicated the following typical electrical cost for industrial power: Michigan (2.48), Arizona (2.27), Missouri (2.05) and Texas (1.49).

In Table 4.2-1, the average product cost without profit is given as $38.41 (1975 dollars) and $53.77 (1980 dollars) per kg for the conventional polysilicon process. This average product costs corresponds to intermediate electrical costs (2.25¢/kw hr for 1975 and 3.15¢/kw hr for 1980). These costs results for the conventional polysilicon process indicate that this Siemen's technology using trichlorosilane to producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

When solar cells come into more widespread use, the capacity of existing polysilicon plants will be exceeded necessitating a new poly plant or plants. Higher capital investment costs will be required for new plants to produce polysilicon by the conventional process. The higher capital investment cost for silicon production in new plants will, of course, appear in higher product cost for polysilicon in terms of increased depreciation, taxes, insurance, etc. The profit will also be higher for a reasonable return on investment for the producing company. Thus, the sales price (product cost with profit) for polysilicon from new plants will be considerably higher than the present price for polysilicon of semiconductor grade produced in existing plants.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities..Table 4.2-2
- Process Design Inputs.....................Table 4.2-3
- Base Case Conditions......................Table 4.2-4
- Raw Material Cost.........................Table 4.2-5
- Utility Cost..............................Table 4.2-6
- Major Process Equipment Cost..............Table 4.2-7
- Production Labor Cost.....................Table 4.2-8
- Plant Investment..........................Table 4.2-9
- Total Product Cost........................Table 4.2-10

TABLE 4.2-1

ESTIMATION OF PRODUCT COST FOR CONVENTIONAL POLYSILICON PROCESS

	Cost $/Kg of Silicon (1975 dollars)	Cost $/Kg of Silicon (1980 dollars)
1. Direct Manufacturing Cost (Direct Costs)......	24.94-30.71	24.92-42.99
Raw Materials		
Direct Operating Labor		
Utilities		
Supervision and Clerical		
Maintenance and Repairs		
Operating Supplies		
Laboratory Charge		
2. Indirect Manufactuing Cost (Fixed Cost).......	1.38	1.93
Depreciation		
Local Taxes		
Insurance		
3. Plant Overhead..............................	3.82	5.35
4. General Expenses............................	5.38	7.54
Administration		
Distribution and Sales		
Research and Development		
5. Product Cost Without Profit..................	35.52-41.29	49.73-57.81
6. Average Product Cost Without Profit..........	38.41	53.77

Basis: The above results are based on a plant constructed in the 1960's. (1965) or earlier) which is fully depreciated. The range for product cost without profit relfects low and high electrical costs (1.5-3¢/kw. hr for 1975 and 2.1-4.2¢/kw hr for 1980). The average product cost without profit reflects intermediate electrical costs (2.25¢/kw hr for 1975 and 3.15¢/kw for 1980).

TABLE 4.2-2

ECONOMIC ANALYSES: PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR CONVENTIONAL POLYSILICON PROCESS

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	●
1. Base Year for Costs	●
2. Appropriate Indices for Costs	●
3. Additional	●
3. Raw Material Costs	●
1. Base Cost/Lb. of Material	●
2. Material Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
4. Utility Costs	●
1. Base Cost for Each Utility	●
2. Utility Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost/Kg Silicon Per Area	●
3. Total Cost/Kg Silicon	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○ Plan
◐ In Progress
● Complete

TABLE 4.2-3

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"

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"

TABLE 4.2-4

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

3. Raw Material Cost
   -Chemical Marketing Reporter
   -January 1975 Value
   -Other Sources

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

5. Update to 1980
   -historically cited 1975 dollars (LSA project)
   -DOE decision to change to 1980 dollars (JPL, 6/22/79)
   -reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

TABLE 4.2-5

RAW MATERIAL COST FOR CONVENTIONAL POLYSILICON PROCESS

Raw Material	Requirement lb/Kg of Silicon	$/lb of Material	Cost $/Kg of Silicon	
1. M.G. Silicon	6.72 (Kg/Kg)	1.0/Kg	6.72	
2. Anhydrous HCl	57.96	.10	5.79	
3. Hydrogen	.828	.96	.79	
4. Caustic (50% NaOH)	53.29	.0382	2.04	
5. $SiCl_4$ (By Product)	46.12	.135	-6.23	(credit)
		TOTAL COST	9.11	(1975 dollars)
			x 1.4	inflation
			12.75	(1980 dollars)

TABLE 4.2-6

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
4.	Process Water	320.9 Gallons	$ .35/M Gal.	.11
5.	Refrigerant (-40°F)	42.1 M BTU	$10.38/MM BTU	.44
6.	Refrigerant (34°F)	32.3 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 (1975 dollars)
				x 1.4 inflation
				19.96 (1980 dollars)

NOTES

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

TABLE 4.2-7

PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR CONVENTIONAL POLYSILICON PROCESS

	Equipment	Purchased Cost, $M
1.	(T1) 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.	(T7) 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.	(T11) TCS Storage Tanks (3)	127.8
12.	(T12) TET/TCS Feed Tanks (3)	54.
13.	(T13) Caustic Storage Tank	106.7
14.	(T14) #1 Distillation Condenser Flash Tank	.85
15.	(T15) Rod Reactor Off Gas Flash Tank	7.2
16.	(H1) 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.	(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	27.5
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 4.2-7 (Continued)

34.	(P1)	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	234.5
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.	(C1)	#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.	(A1)	Molecular Sieves	16.77
61.	(A2)	Fines Separator	4.8
62.	(A3)	Hydrogen Flare	1.
63.	(A4)	Filament Pullers (5)	15. (each)
		TOTAL PURCHASED COST	$19,307.14 (1975 dollars)
			x 1.4 inflation
			$27,030.00 (1980 dollars)

TABLE 4.2-8

PRODUCTION LABOR COST FOR CONVENTIONAL POLYSILICON PROCESS

	Unit Operation	Skilled 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 (1975 dollars) x 1.4 inflation 5.11 (1980 dollars)

*semiskilled

TABLE 4.2-9

ESTIMATION OF PLANT INVESTMENT COST FOR CONVENTIONAL POLYSILICON PROCESS

	Investment ($1000)	
	1975 Plant	1960's Plant
1. DIRECT PLANT INVESTMENT COSTS		
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
6. Process Buildings, Installed	3,303	1,889
1a. 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
2a. SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	21,258	12,147
3. TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	60,391	34,509
4. INDIRECT PLANT INVESTMENT COSTS		
1. Engineering, Overhead, etc.	3,757	2,147
2. Normal Cost. for Floods, Strikes, etc.	9,076	5,186
4a. TOTAL INDIRECT PLANT INVESTMENT COST	12,833	7,333
5. TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	73,224	41,842
6. OVERALL CONTINGENCY, % OF 5 @10%	7,322	4,184
7. FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	80,546	46,026
	Plant Constructed In 1975	Plant Constructed In 1960's (1965 or Earlier)

1980 CE Plant Cost Index = 253 (March)
1975 CE Plant Cost Index = 182
1965 CE Plant Cost Index = 104
1960 CE Plant Cost Index = 102

TABLE 4.2-10

ESTIMATION OF TOTAL PRODUCT COST FOR CONVENTIONAL POLYSILICON PROCESS

	PRODUCT COST, $/KG Si			
	Low 1.5¢/kw hr	High 3¢/kw hr	Intermed. 2.25¢/kw hr	
1. Direct Manufacturing 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 Manaufacturing 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	2.15	2.15	2.15	
2. Distribution and Sales	2.15	2.15	2.15	
3. Research and Development	1.08	1.08	1.08	
6. Total Cost of Product, 4a + 5	35.52	41.29	38.41	(1975 dollars)
	x 1.4	x 1.4	x 1.4	inflation
	49.73	57.81	53.16	(1980 dollars)

Basis: The above results are based on a plant constructed in 1960's (1965 or earlier) which is fully depreciated. The range reflects low and high electrical costs (1.5-3¢/kw hr). Intermediate reflects intermediate electrical cost (2.25¢/kw hr).

4.3 UCC Silane Process for Silicon (Union Carbide Corporation)

The economic analysis activity involves a cost analysis of the process under consideration for the production of silicon. The cost analysis for the particular technology is based on process design results, such as requirements for raw materials and major process equipment necessary to produce the product, from the chemical engineering analysis activity. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silicon by the UCC silane process (Union Carbide Corporation) are presented in Table 4.3-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of $6.90 (1975 dollars) and $9.66 (1980 dollars) per kg. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses.

The product cost represents all cost associated with producing 1 kg of silicon. On top of these costs a producing company will include some profit. The sales price of the product silicon will actually be the sum of the product cost and a profit for the company. The profit is usally measured in terms of rate of return on the capital investment that the company spent in going into the polysilicon business. Two profitability methods which are commonly used are the return on original investment (per cent ROI) and discounted cash flow rate of return (per cent DCF).

The cost and profitability analysis summary for this process are presented in Table 4.3-2. The sales price of polysilicon at various rates of return for both profitability methods (per cent ROI and DCF) is shown in the lower half of the table. The results indicate a sales price of $13 per kg of silicon (1980 dollars) at 15 per cent DCF return on investment.

These cost and profitability results for the UCC silane process indicate that this new technology for producing polysilicon shows good promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities...Table 4.3-3
- Process Design Inputs......................Table 4.3-4
- Base Case Conditions.......................Table 4.3-5
- Raw Material Cost..........................Table 4.3-6
- Utility Cost...............................Table 4.3-7
- Major Process Equipment Cost...............Table 4.3-8
- Production Labor Cost......................Table 4.3-9
- Plant Investment...........................Table 4.3-10
- Total Product Cost.........................Table 4.3-11

The economic analysis provides detailed cost data for raw materials, utilities, labor and major process equipment which are necessary for polysilicon production.

TABLE 4.3-1

ESTIMATION OF PRODUCT COST FOR UCC Silane Process

		Cost $/Kg of Silicon (1975 dollars)	Cost $/Kg of Silicon (1980 dollars)
1.	Direct Manufacturing Cost (Direct Costs)...... Raw Materials Direct Operating Labor Utilities Supervision and Clerical Maintenance and Repairs Operating Supplies Laboratory Charge	4.15	5.81
2.	Indirect Manufactuing Cost (Fixed Cost)....... Depreciation Local Taxes Insurance	1.19	1.67
3.	Plant Overhead................................	0.66	0.92
4.	General Expenses.............................. Administration Distribution and Sales Research and Development	0.90	1.26
5.	Product Cost Without Profit...................	6.90	9.66

TABLE 4.3-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR UCC Silane Process

1. Process....................................UCC Silane Process
2. Plant Size...................................1,000 Metric Tons/year
3. Plant Product................................Silicon
4. Product Form.................................Liquid Phase
5. Plant Investment.............................$10,570,000 / $14,800,000 (1975 dollars) (1980 dollars)

Fixed Capital		$9.19 Mega	$12.87 Mega
Working Capital		$1.38 Mega	$ 1.93 Mega
(15%)	Total	$10.57 Mega	$14.80 Mega
		(1975 dollars)	(1980 dollars)

6. Return on Original Investment, after taxes (%ROI)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% ROI..............	6.90	9.66
5% ROI..............	7.88	11.02
10% ROI..............	8.86	12.39
15% ROI..............	9.84	13.75
20% ROI..............	10.81	15.11
25% ROI..............	11.79	16.47
30% ROI.............	12.77	17.84
40% ROI.............	14.73	20.56

7. Discounted Cash Flow Rate of Return, after taxes (% DCF)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% DCF..............	6.90	9.66
5% DCF..............	7.53	10.54
10% DCF..............	8.22	11.50
15% DCF..............	8.97	12.55
20% DCF..............	9.77	13.65
25% DCF..............	10.60	14.82
30% DCF..............	11.47	16.02
40% DCF..............	13.27	18.53

Based on 10 year project life and 10 year straight line depreciation.

8. Tax Rate (Federal)...................46%

Table 4.3-3
ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR UCC Silane Process

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	●
1. Base Year for Costs	●
2. Appropriate Indices for Costs	●
3. Additional	●
3. Raw Material Costs	●
1. Base Cost/Lb. of Material	●
2. Material Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
4. Utility Costs	●
1. Base Cost for Each Utility	●
2. Utility Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●

Prel. Process Economic Activity	Status
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost/Kg Silicon Per Area	●
3. Total Cost/Kg Silicon	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○ Plan
◐ In Progress
● Complete

TABLE 4.3-4

PROCESS DESIGN INPUTS FOR UCC SILANE PROCESS

1. Raw Material Requirements
   - -M.G. Silicon, silicon tetrachloride, hydrogen, copper catalyst, lime
   - -see table for "Raw Material Cost"
2. Utility
   - -electrical, steam, cooling water, etc.
   - -see table for "Utility Cost"
3. Equipment List
   - -93 pieces of major process equipment
   - -process vessels, heat exchangers, reactor, etc.
4. Labor Requirements
   - -production labor for purification, vaporization, product handling, etc.
   - -see table for "Production Labor Cost"

TABLE 4.3-5

BASE CASE CONDITIONS FOR
UCC SILANE RPOCESS

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

3. Raw Material Cost

   -Chemical Marketing Reporter
   -January 1975 Value
   -Raw Material Cost Index for Industrial Chemicals
   -1975 Cost Index Value = 206.9 (Wholesale Price Index, Producer Price Index)

4. Labor Cost

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

5. Update to 1980

   -historically cited 1975 dollars (LSA project)
   -DOE decision to change to 1980 dollars (JPL,6/22/79)
   -reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

TABLE 4.3-6

RAW MATERIAL COST FOR UCC SILANE PROCESS

	Raw Material	Requirement lb/KG of Si	$/lb of Material	Cost $/KG of Si
1.	M.G. Silicon (Si)	2.60	0.535	1.391
2.	Silicon Tetrachloride ($SiCl_4$, make-up)	2.76	0.135	0.373
3.	Liquid Hydrogen (H_2, make-up)	0.032	1.84	0.059
4.	Copper Catalyst (Cu)	0.051	0.922	0.047
5.	Hydrate Lime ($Ca(OH)_2$)	2.43	0.015 (33.2$/ton)	0.036
			TOTAL	1.906 (1975 dollars)
				x 1.4 inflation
				2.668 (1980 dollars)

TABLE 4.3-7

UTILITY COST FOR UCC SILANE PROCESS

	Utility	Requirement/KG of Silicon	Cost of Utility	Cost $/KG of Silicon
1.	Electricity	3.050 KW	0.0324 $/KW-HR	0.0988
2.	Steam	172.200 lbs.	1.35 $/klb	0.2325
3.	Cooling Water	525.000 gallons	0.09 $/kgal	0.0473
4.	Process Water	0.0709 gallons	0.405$/kgal	0.0001
5.	Refrigerant	968.000 Btu	10.50 $/MBtu	0.0102
6.	Fuel	27,100.00 Btu	1.40 $/MBtu	0.0379
			TOTAL	0.43 (1975 dollars)
				x 1.4 inflation
				0.60 (1980 dollars)

Note:

$k = \text{kilo} = 10^3$
$M = \text{mega} = 10^6$

TABLE 4.3-8

PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR
UCC SILANE PROCESS

	Equipment	Purchased Cost, $1000
1.	(D-01) Crude TCS/STC Stripping Column	5.5
2.	(D-02) TCS/STC Distillation Column	32.6
3.	(D-03) DCS/TCS Distillation Column	61.6
4.	(D-04) Silane Distillation Column	50.3
5.	(R-01) Hydrogenation Reactor	82.6
6.	(R-) DCS Redistribution Reactor	19.2
7.	(R-03) TCS Redistribution Teactor	17.3
8-9.	(R-04) Sludge Neutralization Reactor	10.3
10.	(H-01) Liquid H_2 Vaporizer (Provided by Vendor)	------
11.	(H-02) STC Cooler	26.4
12.	(H-03) Quench Condenser	22.6
13.	(H-04) Recycle STC Vaporizer	3.3
14.	(H-05) Recycle STC Superheater	35.0
15.	(H-06) Recycle H_2 Heater	10.8
16.	(H-07) Stripper Reboiler	1.5
17.	(H-08) Stripper Condenser	1.4
18.	(H-09) TCS/STC Reboiler	8.6
19.	(H-10) TCS/STC Condenser	44.5
20.	(H-11) DCS/TCS Reboiler	8.2
21.	(H-12) DCS/TCS Condenser	16.2
22.	(H-13) DCS Cooler	1.5
23.	(H-14) TCS Cooler	3.0

TABLE 4.3-8 (Continued)

24.	(H-15) Silane Reboiler	1.3
25.	(H-16) Silane Condenser	2.6
26.	(H-17) Silane Vaporizer/Superheater	2.4
27.	(H-18) Pyrolysis Hydrogen Cooler	4.1
28.	(H-19) First Stage H_2 Intercooler	3.6
29.	(H-20) Second Stage H_2 Intercooler	3.6
30.	(C-01) Pneumatic Conveying Fan	1.6
31.	(C-02) Recycle H_2 Blower	4.7
32.	(C-03) First Stage H_2 Compressor	9.7
33.	(C-04) Second Stage H_2 Compressor	9.7
34.	(C-05) Third Stage H_2 Compressor	9.7
35.	(P-01) Quench Contactor Pump	2.4
36.	(P-03) Recycle STC Pump	15.0
37.	(P-04) TCS Distillate Pump	19.8
38.	(P-05) DCS Distillate Pump	11.3
39.	(P-06) Lime Tank Pump	2.0
40.	(T-01) Crude TCS/STC Storage Tank	39.0
41.	(T-02) STC Storage Tank	17.0
42.	(T-03) Liquid H_2 Storage (Provided By Vendor)	———
43.	(T-04) Waste Settler Tank	27.0
44.	(T-05) Waste Chloride Tank	1.8
45.	(T-06) Quench Condenser Receiver	8.8
46.	(T-07) Recycle H_2 Receiver	7.2

TABLE 4.3-8 (Continued)

47.	(T-08) Stripper Reflux pot	1.2
48.	(T-09) TCS/STC Reflux pot	6.1
49.	(T-10) DCS/TCS Reflux pot	11.2
50.	(T-11) A, B Silane Shift Tank (two)	20.6 ea.
51.	(T-13) Pyrolysis H_2 Receiver	7.9
52.	(T-14) Lime Make-up Tank	5.7
53.	(T-15) Sludge Pump Tank	11.5
54.	(B-01) M. G. Silicon Storage Hopper	12.2
55-56.	(B-04) Pyrolysis Dust Bin	1.7
57.	(F-01) Crude TCS/STC Filter	0.7
58.	(F-02) Waste Hydroxide Filter	5.0
59.	(F-03) Pyrolysis H_2 Filter	0.7
60.	(F-04) M. G. Silicon Unloading Filter	1.6
61.	(S-01) M. G. Silicon Unloading Cyclone	1.4
62.	(S-02) Double Shell Blender	13.0
63.	(S-03) M. G. Silicon Loak Hopper	5.8
64.	(U-01) Quench Contactor Ejector	1.3
65.	(U-02) Lime Tank Agitator	1.3
66.	(U-03) Vent Gas Combustor	6.3
67.	(U-04) Vent Gas Ejector	1.3
68.	(R-05) Silane Pyrolysis Reactor (six)	46.8 ea.
69.	(X-01) Melters (six)	53.0 ea.
70.	(B-05) Powder Hoppers (two)	19.9 ea.
71.	(X-02) Hydrogen Cooler	4.1

TABLE 4.3-8 (Continued)

72.	(X-03) Hydrogen Blower	2.5
73.	(X-04) Dust Filter	0.8
74.	(X-05) Star Valve (six)	1.2 ea.
75.	(X-06) Conveyor	8.3
76.	(X-07) Drum Loader	16.6
	TOTAL	1481.9 (1975 dollars)
		x 1.4 inflation
		2074.7 (1980 dollars)

TABLE 4.3-9

PRODUCTION LABOR COST FOR UCC SILANE PROCESS

Section/ Unit Operation	Skilled Labor Man-Hrs/KG of Si	Semiskilled Labor Man-Hrs/KG of Si	Cost $/KG of Si
1. Hydrogenation	0.00745	0.000745	0.0879
2. Silane	0.02230	---------	0.1539
3. Pyrolysis	0.02980	---------	0.2056
4. Waste Treatment	0.00745	---------	0.0514
5. Hydrogen Compression	0.00745	---------	0.0514
		TOTAL	0.55 (1975 dollars) x 1.4 inflation 0.77 (1980 dollars)

TABLE 4.3-10

ESTIMATION OF PLANT INVESTMENT FOR UCC SILANE PROCESS

		Investment $1000	
1.	DIRECT PLANT INVESTMENT COSTS		
	1. Major Process Equipment Cost	1,481.9	
	2. Installation of Major Process Equipment	637.2	
	3. Process Piping, Installed	1,096.6	
	4. Instrumentation, Installed	281.6	
	5. Electrical, Installed	148.2	
	6. Process Buildings, Installed	148.2	
1a.	SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	3,793.7	
2.	OTHER DIRECT PLANT INVESTMENT COSTS		
	1. Utilities, Installed	711.3	
	2. General Services, Site Development, Fire Protection, etc.	177.8	
	3. General Buildings, Offices, Shops, etc.	207.5	
	4. Receiving, Shipping Facilities	311.2	
2a.	SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	1,407.8	
3.	TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	5,201.5	
4.	INDIRECT PLANT INVESTMENT COSTS		
	1. Engineering, Overhead, etc.	815.0	
	2. Normal Cont. for Floods, Strikes, etc.	1,052.1	
4a.	TOTAL INDIRECT PLANT INVESTMENT COST	1,867.1	
5.	TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	7,068.6	
6.	OVERALL CONTINGENCY, % of 5	2,120.6	
7.	FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	9,189.2	(1975 dollars)
		x 1.4	inflation
		12,864.9	(1980 dollars)

TABLE 4.3-11

ESTIMATION OF TOTAL PRODUCT COST FOR UCC SILANE PROCESS

		$/KG of Si
1.	Direct Manufacturing Cost (Direct Charges)	
	1. Raw Materials	1.906
	2. Direct Operating Labor	0.550
	3. Utilities	0.427
	4. Supervision and Clerical	0.083
	5. Maintenance and Repairs	0.919
	6. Operating Supplies	0.184
	7. Laboratory Charge	0.083
2.	Indirect Manufacturing Cost (Fixed Charges)	
	1. Depreciation	0.919
	2. Local Taxes	0.184
	3. Insurance	0.092
3.	Plant Overhead	0.656
4.	By-Product Credit	-----
4a.	Total Manufacturing Cost, 1 + 2 + 3 + 4	6.003
5.	General Expenses	
	1. Administration	0.360
	2. Distribution and Sales	0.360
	3. Research and Development	0.180
6.	Total Cost of Product, 4a + 5	6.903 (1975 dollars) x 1.4 inflation 9.664 (1980 dollars)

4.4 BCL Process for Silicon - Case A (Battelle Columbus Laboratories)

The economic analysis activity involves a cost analysis of the process under consideration for the production of silicon. The cost analysis for the particular technology is based on process design results, such as requirements for raw materials and major process equipment necessary to produce the product, from the chemical engineering analysis activity. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silicon by the BCL process-Case A (Battelle Columbus Laboratories) are presented in Table 4.4-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of \$8.63 (1975 dollars) and \$12.08 (1980 dollars) per kg. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses.

The product cost represents all cost associated with producing silicon. On top of these costs a producing company will include some profit. The sales price of the product silicon will actually be the sum of the product cost and a profit for the company. The profit is usually measured in terms of rate of return on the capital investment that the company spent in going into the polysilicon business. Two profitability methods which are commonly used are the return on original investment (per cent ROI) and discounted cash flow rate of return (per cent DCF).

The cost and profitability analysis summary for this process are presented in Table 4.4-2. The sales price of polysilicon at various rates of return for both profitability methods (per cent ROI and DCF) is shown in the lower half of the table. The results indicate a sales price of \$13.28 per kg of silicon (1980 dollars) at 5 per cent DCF return on investment after taxes.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities..Table 4.4-3
- Process Design Inputs.....................Table 4.4-4
- Base Case Conditions......................Table 4.4-5
- Raw Material Cost.........................Table 4.4-6
- Utility Cost..............................Table 4.4-7
- Major Process Equipment Cost..............Table 4.4-8
- Production Labor Cost.....................Table 4.4-9
- Plant Investment..........................Table 4.4-10
- Total Product Cost........................Table 4.4-11

These cost and profitability results for the BCL process-Case A indicate that this new technology for producing polysilicon shows promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

TABLE 4.4-1

ESTIMATION OF PRODUCT COST FOR BCL PROCESS - CASE A

	Cost $/Kg of Silicon (1975 dollars)	Cost $/Kg of Silicon (1980 dollars)
1. Direct Manufacturing Cost (Direct Costs)......	5.21	7.29
Raw Materials		
Direct Operating Labor		
Utilities		
Supervision and Clerical		
Maintenance and Repairs		
Operating Supplies		
Laboratory Charge		
2. Indirect Manufactuing Cost (Fixed Cost).......	1.62	2.27
Depreciation		
Local Taxes		
Insurance		
3. Plant Overhead...............................	0.68	0.95
4. General Expenses.............................	1.12	1.57
Administration		
Distribution and Sales		
Research and Development		
5. Product Cost Without Profit..................	8.63	12.08

TABLE 4.4-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR BCL PROCESS-CASE A

1. Process.................................BCL Process-Case A
2. Plant Size..............................1,000 Metric Tons/year
3. Plant Product...........................Silicon
4. Product Form............................Silicon Granules
5. Plant Investment........................$14,340,000 /$20,070,000 (1975 dollars) (1980 dollars)

Fixed Capital		$12.47Mega	$17.45 Mega
Working Capital		$ 1.87Mega	$ 2.62 Mega
(15%)	Total	$14.34Mega	$20.07 Mega
		(1975 dollars)	(1980 dollars)

6. Return on Original Investment, after taxes (%ROI)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% ROI..............	8.63	12.08
5% ROI..............	9.96	13.94
10% ROI..............	11.28	15.80
15% ROI..............	12.61	17.65
20% ROI..............	13.94	19.51
25% ROI..............	15.27	21.37
30% ROI.............	16.59	23.23
40% ROI.............	19.25	26.95

7. Discounted Cash Flow Rate of Return, after taxes (% DCF)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% DCF..............	8.63	12.08
5% DCF..............	9.48	13.28
10% DCF..............	10.42	14.59
15% DCF..............	11.44	16.02
20% DCF..............	12.52	17.53
25% DCF..............	13.65	19.11
30% DCF.............	14.82	20.75
40% DCF..............	17.27	24.18

Based on 10 year project life and 10 year straight line depreciation.

8. Tax Rate (Federal)........................

TABLE 4.4-3

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR BCL PROCESS-CASE A

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	●
1. Base Year for Costs	●
Appropriate Index for	●
[illegible]	●
3. Raw Material Cost	●
1. Base Cost of Raw Material	●
Kg of Material	●
Total Cost/Kg of Silicon	●
4. Utility Cost	●
1. Base Cost for Each Utility	●
2. Quantity in [illegible]	●
3. Total Cost/Kg of Silicon	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●

Prel. Process Economic Activity	Status
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost Kg Silicon Per Area	●
3. Total Cost/Kg Silicon	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○ Plan
◐ In Progress
● Complete

TABLE 4.4-4

PROCESS DESIGN INPUTS FOR BCL PROCESS - Case A

1. Raw Material Requirements
   - -Silicon tetrachloride, zinc, lime, argon and nitrogen
   - -see table for "Raw Material Cost"

2. Utility
   - -electricity, steam, cooling water and process water
   - -see table for "Utility Cost"

3. Equipment List
   - -82 plus pieces of major process equipment
   - -process vessels, heat exchangers, reactor, etc.

4. Labor Requirements
   - -production labor for purification, deposition, electrolysis, etc.
   - -see table for "Production Labor Cost"

TABLE 4.4-5
BASE CASE CONDITION FOR BCL PROCESS-CASE A

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

3. Raw Material Cost

   -Chemical Marketing Reporter
   -January 1975 Value
   -Raw Material Cost Index for Industrial Chemicals
   -1975 Cost Index Value [illegible] (Wholesale Price Index, Producer Price Index)

4. Labor Cost

   -Average for Chemical Petroleum, Coal and Allied Industries (1975)
   -Skilled $6.90/hr

5. Update to 1980

   -historically cited 1975 dollars (LSA project)
   -DOE decision to change to 1980 dollars (JPL, 6/22/79)
   -reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

Table 4.4-6

RAW MATERIAL COST FOR BCL PROCESS-CASE A

	Raw Material	Requirement lb/KG of Si	$/lb of Material	Cost $/KG of Si
1.	Silicon Tetrachloride ($SiCl_4$)	15.68	0.135	2.117
2.	Zinc (Zn)	0.54	0.38	0.205
3.	Hydrate Lime ($Ca(OH)_2$)	2.85	0.015	0.043
4.	Argon (Ar)	3.1 SCF	0.016/SCF	0.050
5.	Nitrogen (N_2)	7.6 SCF	0.003/SCF	0.023
			Sub Total	2.438
6.	Chlorine (Cl_2)	-10.46[1]	0.0332	-0.347
			TOTAL	2.091 (1975 dollars) x 1.4 inflation 2.927 (1980 dollars)

Note:

[1] This number is the result of by-product rate minus reactor chlorination rate, i.e., 11.12 - 0.66 lb. of Cl_2/KG Si.

Table 4.4-7
UTILITY COST FOR BCL PROCESS-CASE A

	Utility	Requirement/KG of Silicon	Cost of Utility	Cost $/KG of Silicon
1.	Electricity	30.92 kw-hr	0.0324 $/kw-hr	1.0018
2.	Steam	9.67 pounds	1.35 $/klb	0.0131
3.	Cooling Water	37.88 Gallons	0.09 $/kgal	0.0034
4.	Process Water	24.20 Gallons	0.405 $/kgal	0.0098
5.	Refrigerant	2.38 MBtu	10.50 $/MBtu	0.0250
			TOTAL	1.0531 (1975 dollars) x 1.4 inflation 1.4743 (1980 dollars)

Note:

k = kilo = 10^3
M = mega = 10^6

TABLE 4.4-8

ESTIMATED COST OF MAJOR PROCESS EQUIPMENT FOR BCL PROCESS-CASE A

	Equipment	Purchased Cost, $1,000
1.	(D-01) Light End Distillation Column	55.6
2.	(D-02) Heavy End Distillation Column	55.6
3.	(A-01) Primary $SiCl_4$ Vent Scrubber	0.8
4.	(A-02) Final $SiCl_4$ Vent Scrubber	11.1
5.	(H-01) L. E. Column Feed Heater	7.8
6.	(H-02) L. E. Column Reboiler	2.2
7.	(H-03) L. E. Column Condenser	2.3
8.	(H-04) H. E. Column Feed Heater	7.8
9.	(H-05) H. E. Column Reboiler	2.4
10.	(H-06) H. E. Column Condenser	2.3
11.	(H-07) $SiCl_4$ Vent Condenser	11.8
12.	(H-08) $SiCl_4$ Vaporizer	6.7
13.	(H-09) Reactor Condensers (2)	190.3
14.	(H-10) Reactor $ZnCl_2$ Strippers (2)	27.9
15.	(H-11) $SiCl_4$ Condenser	20.5
16.	(H-12) Cell $ZnCl_2$ Stripper	10.9
17.	(H-13) Therminol Cooler (Cold Circuit)	3.8
18.	(H-14) Therminol Cooler (Hot Circuit)	9.1
19.	(H-15) Start-up Heater	9.6
20.	(H-16) Silicon Product Coolers (2)	7.7
20a.	(H-17) Chlorination Cooler	15.9
20b.	(H-18) Cell Gas Cooler	18.7
21.	(T-01) $SiCl_4$ Storage Tank	33.6
22.	(T-02) $SiCl_4$ Emergency Storage Tank	33.6
23.	(T-03) L. E. Column Reflux Drum	6.7

TABLE 4.4-8 (Continued)

24.	(T-04) Surge Tank	19.0
25.	(T-05) Sump Tank	19.0
26.	(T-06) H. E. Column Reflux Drum	6.7
27.	(T-07) Pure $SiCl_4$ Storage Tank	28.8
28.	(T-08) Electrolysis Feed Tank	46.0
29.	(T-09) Molten Zinc Storage Tank	86.9
30.	(T-10) Therminol Head Tank	3.8
31.	(T-11) Therminol Drain Down Tank	5.3
32.	(T-12) Chlorine Supply Tank	2.4
33.	(T-13) Lime Solution Storage Tank	6.8
34.	(P-01) Purification Feed Pump	3.7
35.	(P-02) L. E. Column Feed Pump	8.4
36.	(P-03) L. E. Column Reflux Pump	8.4
37.	(P-04) Surge Tank Pump	9.8
38.	(P-05) Sump Pump	3.7
39.	(P-06) L. E. Column Bottom Pump	12.0
40.	(P-07) H. E. Column Reflux Pump	8.4
41.	(P-08) H. E. Column Bottom Pump	10.9
42.	(P-09) $SiCl_4$ Vaporizer Feed Pump	4.8
43.	(P-10) Reactor Condenser Circulation Pumps (2)	14.4
44.	(P-11) Cold Circuit Pump	6.7
45.	(P-12) Hot Circuit Pump	13.9
46.	(P-13) Primary Scrubber Recirculation Pump	0.9
47.	(P-14) Primary Scrubber Lower-loop Recirculation Pump	1.4
48.	(P-15) Primary Scrubber Upper-loop Recirculation Pump	1.5
49.	(P-16) Lime Solution Metering Pump	1.4

TABLE 4.4-8 (Continued)

50.	(F-01) L. E. Column Feed Filter	0.9
51.	(F-02) L. E. Column Reflux Filter	0.9
52.	(F-03) H. E. Column Feed Filter	0.9
53.	(F-04) H. E. Column Reflux Filter	0.9
54.	(F-05) Therminol Cooler Blower Filter	0.7
55.	(R-01) Fludized Bed Reactors (2)	197.1
56.	(FN-01) Furnaces (2)	354.2
57.	(B-01) Seed Addition Hoppers (2)	9.6
58.	(B-02) Si Product Hoppers (4)	14.4
59.	(B-03) Zinc Hopper	2.4
60.	(C-01) Therminol Cooler Blower	4.8
61.	(C-02) Scrubber Vent Blower	5.4
62.	(E-01) Eductors (2)	1.3
63.	(EC-01) Electrolysis Cells (6)	441.6
64.	(PW-01) Power Supply and Bus	105.9
65.	(VP-01) Zinc Vaporizers (2)	144.0
	TOTAL	2,177.7 (1975 dollars) x 1.4 inflation 3,048.8 (1980 dollars)

TABLE 4.4-9

PRODUCTION LABOR COST FOR BCL PROCESS-CASE A

	Section	Labor Man-Hr/Kg Si	Labor Cost $/Man-Hr	Cost $/Kg Si
1.	Purification	0.01402	6.90	0.0968
2.	Deposition	0.01402	6.90	0.0968
3.	Electrolysis	0.02103	6.90	0.1451
4.	Waste Treatment	0.00701	6.90	0.0484
5.	Product Handling	0.00701	6.90	0.0484
			TOTAL	0.4355 (1975 dollars)
				x 1.4 inflation
				0.6097 (1980 dollars)

Note: Costs are 1975 Dollars

TABLE 4.4-10

ESTIMATION OF PLANT INVESTMENT FOR BCL PROCESS-CASE A

	Investment $1000
1. DIRECT PLANT INVESTMENT COSTS	
1. Major Process Equipment Cost	2,177.7
2. Installation of Major Process Equipment	936.4
3. Process Piping, Installed	1,611.5
4. Instrumentation, Installed	413.8
5. Electrical, Installed	217.8
6. Process Buildings, Installed	217.8
1a. SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	5,574.9
2. OTHER DIRECT PLANT INVESTMENT COSTS	
1. Utilities, Installed	[illegible]
2. General Service, Site Development, Fire Protection, etc.	[illegible]
3. General Buildings, Offices, Shops, etc.	304.[illegible]
4. Receiving, Shipping Facilities	457.3
2a. SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	2,068.8
3. TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	7,643.7
4. INDIRECT PLANT INVESTMENT COSTS	
1. Engineering, overhead, etc.	1,197.[illegible]
2. Normal Cont. for Floods, Strikes, etc.	1,546.[illegible]
4a. TOTAL INDIRECT PLANT INVESTMENT COST	2,74[illegible]
5. TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	1[illegible],387.6
6. OVERALL CONTINGENCY, % of 5	2,07[illegible]
7. [illegible] INVESTMENT FOR PLANT, 5 + 6	[illegible],465.[illegible] (1975 [illegible]) x 1.4 inflation 17,451.2 (1980 dollars)

TABLE 4.4-11

ESTIMATION OF TOTAL PRODUCT COST FOR BCL PROCESS - CASE A

	$/KG of Si
1. Direct Manufacturing Cost (Direct Charges)	
1. Raw Materials	2.091
2. Direct Operating Labor	0.436
3. Utilities	1.053
4. Supervision and Clerical	0.065
5. Maintenance and Repairs	1.247
6. Operating Supplies	0.249
7. Laboratory Charge	0.065
2. Indirect Manaufacturing Cost (Fixed Charges)	
1. Depreciation	1.247
2. Local Taxes	0.249
3. Insurance	0.125
3. Plant Overhead	0.675
4. By-Product Credit	-----
4a. Total Manufacturing Cost, 1 + 2 + 3 + 4	7.501
5. General Expenses	
1. Administration	0.450
2. Distribution and Sales	0.450
3. Research and Development	0.225
6. Total Cost of Product, 4a + 5	8.626 (1975 dollars) x 1.4 inflation 12.076 (1980 dollars)

4.5 BCL Process for Silicon - Case B (Battelle Columbus Laboratories)

The economic analysis activity involves a cost analysis of the process under consideration for the production of silicon. The cost analysis for the particular technology is based on process design results, such as requirements for raw materials and major process equipment necessary to produce the product, from the chemical engineering analysis activity. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silicon by the BCL process - Case B (Battelle Columbus Laboratories) are presented in Table 4.5-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of \$7.91 (1975 dollars) and \$11.07 (1980 dollars) per kg. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses.

The product cost represents all cost associated with producing silicon. On top of these costs a producing company will include some profit. The sales price of the product silicon will actually be the sum of the product cost and a profit for the company. The profit is usually measured in terms of rate of return on the capital investment that the company spent in going into the polysilicon business. Two profitability methods which are commonly used are the return on original investment (per cent ROI) and discounted cash flow rate of return (per cent DCF).

The cost and profitability analysis summary for this process are presented in Table 4.5-2. The sales price of polysilicon at various rates of return for both profitability methods (per cent ROI and DCF) is shown in the lower half of the table. The results indicate a sales price of \$13.14 per kg of silicon (1980 dollars) at 10 per cent DCF return on investment.

These cost and profitability results for the BCL process-Case B indicate that this new technology for producing polysilicon shows promise for meeting the cost goal of \$14 per kg of silicon material (1980 dollars) for solar cells.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interst. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities..Table 4.5-3
- Process Design Inputs.....................Table 4.5-4
- Base Case Conditions......................Table 4.5-5
- Raw Material Cost.........................Table 4.5-6
- Utility Cost..............................Table 4.5-7
- Major Process Equipment Cost..............Table 4.5-8
- Production Labor Cost.....................Table 4.5-9
- Plant Investment..........................Table 4.5-10
- Total Product Cost........................Table 4.5-11

TABLE 4.5-1

ESTIMATION OF PRODUCT COST FOR BCL PROCESS - CASE B

	Cost $/Kg of Silicon (1975 dollars)	Cost $/Kg of Silicon (1980 dollars)
1. Direct Manufacturing Cost (Direct Costs)......	4.94	6.92
Raw Materials		
Direct Operating Labor		
Utilities		
Supervision and Clerical		
Maintenance and Repairs		
Operating Supplies		
Laboratory Charge		
2. Indirect Manufactuing Cost (Fixed Cost).......	1.33	1.86
Depreciation		
Local Taxes		
Insurance		
3. Plant Overhead............................	.61	.85
4. General Expenses..........................	1.03	1.44
Administration		
Distribution and Sales		
Research and Development		
5. Product Cost Without Profit...................	7.91	11.07

TABLE 4.5-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR BCL PROCESS- CASE B

1. Process.................................BCL Process - Case B
2. Plant Size..............................1,000 Metric Tons/year
3. Plant Product...........................Silicon
4. Product Form............................Silicon Granules
5. Plant Investment........................$11,790,000 /$16,500,000 (1975 dollars) (1980 dollars)

Fixed Capital		$10.25Mega	$14.35Mega
Working Capital		$ 1.54Mega	$ 2.15Mega
(15%)	Total	$11.79Mega	$16.50Mega
		(1975 dollars)	(1980 dollars)

6. Return on Original Investment, after taxes (%ROI)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% ROI..............	7.91	11.07
5% ROI..............	9.00	12.60
10% ROI..............	10.09	14.13
15% ROI..............	11.18	15.66
20% ROI..............	12.28	[illegible]
25% ROI..............	13.37	18.71
30% ROI..............	14.46	20.24
40% ROI..............	16.64	23.29

7. Discounted Cash Flow Rate of Return, after taxes (% DCF)

	Sales Price $/Kg of Silicon (1975 dollars)	Sales Price $/Kg of Silicon (1980 dollars)
0% DCF..............	7.91	11.07
5% DCF..............	8.61	12.05
10% DCF..............	9.30	13.14
15% DCF..............	10.72	14.31
20% DCF..............	[illegible]	[illegible]
25% DCF..............	12.04	16.85
30% DCF..............	13.01	18.20
40% DCF..............	15.02	[illegible]

Based on 10 year project life and 10 year straight line depreciation.

8. Tax Rate (Federal).......................................48%

TABLE 4.5-3

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR BCL PROCESS-CASE B

	Prel. Process Economic Activity	Status
1.	Process Design Inputs	●
	1. Raw Material Requirements	●
	2. Utility Requirements	●
	3. Equipment List	●
	4. Labor Requirements	●
	Specify Base Case Conditions	●
	1. Base Year for Costs	●
	2 Appropriate Indices for Costs	●
	Additional	●
3.	Raw Material Costs	●
	1. Base Cost Lb. of Material	●
	Material Cost Kg of Silicon	●
	Total Cost/Kg of Silicon	●
4.	Utility Costs	●
	1. Base Cost for Each Utility	●
	2 Utility Cost/Kg Silicon	●
	3. Total Cost/Kg of Silicon	●
5.	Major Process Equipment Cost	●
	1. Individual Equipment Cost	●
	2. Cost Index Adjustment	●

	Prel. Process Economic Activity	Status
6.	Production Labor Costs	●
	1. Base Cost Per Man Hour	●
	2. Cost/Kg Silicon Per Area	●
	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)	●
	Estimation of Total Product Cost	●
	1. Direct Manufacturing Cost	●
	Indirect Manufacturing Cost	●
	3. Plant Overhead	●
	4. By-Product Credit	●
	General Expenses	●
	Total Cost of Product	●

○ Plan
◐ In Progress
● Complete

TABLE 4.5-4

PROCESS DESIGN INPUTS FOR BCL PROCESS - CASE B

1. Raw Material Requirements
   - -Silicon tetrachloride, zinc, lime, argon and nitrogen
   - -see table for "Raw Material Cost"
2. Utility
   - -electricity, steam, cooling water and process water
   - -see table for "Utility Cost"
3. Equipment List
   - -70 plus pieces of major process equipment
   - -process vessels, heat exchangers, reactor, etc.
4. Labor Requirements
   - -production labor for purification, deposition, electrolysis, etc.
   - -see table for "Production Labor Cost"

TABLE 4.5-5
BASE CASE CONDITION FOR BCL PROCESS- CASE B

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

3. Raw Material Cost

    -Chemical Marketing Reporter
    -January 1975 Value
    -Raw Material Cost Index for Industrial Chemicals
    -1975 Cost Index Value = 206.9 (Wholesale Price Index, Producer Price Index)

4. Labor Cost

    -Average for Chemical Petroleum, Coal and Allied Industries (1975)
    -Skilled $6.90/hr

5. Update to 1980

    -historically cited 1975 dollars (LSA project)
    -DOE decision to change to 1980 dollars (JPL, 6/22/79)
    -reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
    -inflation factor of 1.4 to be used (JPL, 6/22/79)

Table 4.5-6

RAW MATERIAL COST FOR BCL PROCESS-CASE B

	Raw Material	Requirement lb/KG of Si	$/lb of Material	Cost $/KG of Si
1.	Silicon Tetrachloride ($SiCl_4$)	15.68	0.135	2.117
2.	Zinc (Zn)	0.54	0.38	0.205
3.	Hydrate Lime ($Ca(OH)_2$)	2.85	0.015	0.043
4.	Argon (Ar)	3.1 SCF	0.016/SCF	0.050
5.	Nitrogen (N_2)	7.6 SCF	0.003/SCF	0.023
			Sub Total	2.438
6.	Chlorine (Cl_2)	-10.46[1]	0.0332	-0.347
			TOTAL	2.091 (1975 dollars) x 1.4 inflation 2.927 (1980 dollars)

Note:

1. This number is the result of by-product rate minus reactor chlorination rate, i.e., 11.12 - 0.66 lb. of Cl_2/KG Si.

Table 4.5-7
UTILITY COST FOR BCL PROCESS-CASE B

	Utility	Requirement/KG of Silicon	Cost of Utility	Cost $/KG of Silicon
1.	Electricity	30.92 KW-HR	0.0324 $/KW-HR	1.0018
2.	Steam	9.67 pounds	1.35 $/Mlb	0.0131
3.	Cooling Water	37.88 Gallons	0.09 $/Mgal	0.0034
4.	Process Water	24.20 Gallons	0.405 $/Mgal	0.0098
5.	Refrigerant	2.38 MBtu	10.50 $/MMBtu	0.0250
			TOTAL	1.0531 (1975 dollars) x 1.4 inflation 1.4743 (1980 dollars)

TABLE 4.5-8

ESTIMATED COST OF MAJOR PROCESS EQUIPMENT FOR BCL PROCESS-CASE B

	Equipment	Purchased Cost, $1,000
1.	(D-01) Light End Distillation Column	55.6
2.	(D-02) Heavy End Distillation Column	55.6
3.	(A-01) Primary $SiCl_4$ Vent Scrubber	0.8
4.	(A-02) Final $SiCl_4$ Vent Scrubber	11.1
5.	(H-01) L. E. Column Feed Heater	7.8
6.	(H-02) L. E. Column Reboiler	2.2
7.	(H-03) L. E. Column Condenser	2.3
8.	(H-04) H. E. Column Feed Heater	7.8
9.	(H-05) H. E. Column Reboiler	2.4
10.	(H-06) H. E. Column Condenser	2.3
11.	(H-07) $SiCl_4$ Vent Condenser	11.8
12.	(H-08) $SiCl_4$ Vaporizer	6.7
13.	(H-09) Reactor Condensers (2)	144.2
14.	(H-10) Reactor $ZnCl_2$ Strippers (2)	21.1
15.	(H-11) $SiCl_4$ Condenser	20.5
16.	(H-12) Cell $ZnCl_2$ Stripper	10.9
17.	(H-13) Therminol Cooler (Cold Circuit)	3.8
18.	(H-14) Therminol Cooler (Hot Circuit)	9.1
19.	(H-15) Start-up Heater	9.6
20.	(H-16) Silicon Product Coolers (2)	5.8
20a.	(H-17) Chlorination Cooler	15.9
20b.	(H-18) Cell Gas Cooler	18.7
21.	(T-01) $SiCl_4$ Storage Tank	33.6
22.	(T-02) $SiCl_4$ Emergency Storage Tank	33.6
23.	(T-03) L. E. Column Reflux Drum	6.7

TABLE 4.5-8 (Continued)

24.	(T-04) Surge Tank	19.0
25.	(T-05) Sump Tank	19.0
26.	(T-06) H. E. Column Reflux Drum	6.7
27.	(T-07) Pure $SiCl_4$ Storage Tank	28.8
28.	(T-08) Electrolysis Feed Tank	46.0
29.	(T-09) Molten Zinc Storage Tank	86.9
30.	(T-10) Therminol Head Tank	3.8
31.	(T-11) Therminol Drain Down Tank	5.3
32.	(T-12) Chlorine Supply Tank	2.4
33.	(T-13) Lime Solution Storage Tank	6.8
34.	(P-01) Purification Feed Pump	3.7
35.	(P-02) L. E. Column Feed Pump	8.4
36.	(P-03) L. E. Column Reflux Pump	8.4
37.	(P-04) Surge Tank Pump	9.8
38.	(P-05) Sump Pump	3.7
39.	(P-06) L. E. Column Bottom Pump	12.0
40.	(P-07) H. E. Column Reflux Pump	8.4
41.	(P-08) H. E. Column Bottom Pump	10.9
42.	(P-09) $SiCl_4$ Vaporizer Feed Pump	4.8
43.	(P-10) Reactor Condenser Circulation Pumps (2)	10.9
44.	(P-11) Cold Circuit Pump	6.7
45.	(P-12) Hot Circuit Pump	13.9
46.	(P-13) Primary Scrubber Recirculation Pump	0.9
47.	(P-14) Primary Scrubber Lower-loop Recirculation Pump	1.4
48.	(P-15) Primary Scrubber Upper-loop Recirculation Pump	1.5
49.	(P-16) Lime Solution Metering Pump	1.4

TABLE 4.5-8 (Continued)

50.	(F-01) L. E. Column Feed Filter	0.9	
51.	(F-02) L. E. Column Reflux Filter	0.9	
52.	(F-03) H. E. Column Feed Filter	0.9	
53.	(F-04) H. E. Column Reflux Filter	0.9	
54.	(F-05) Therminol Cooler Blower Filter	0.7	
55.	(R-01) Fludized Bed Reactors	149.4	
56.	(FN-01) Furnaces	268.5	
57.	(B-01) Seed Addition Hoppers	7.3	
58.	(B-02) Si Product Hoppers (4)	14.4	
59.	(B-03) Zinc Hopper	2.4	
60.	(C-01) Therminol Cooler Blower	4.8	
61.	(C-02) Scrubber Vent Blower	5.4	
62.	(E-01) Eductors (2)	1.3	
63.	(EC-01) Electrolysis Cells (2)	286.5	
64.	(PW-01) Power Supply and Bus	105.9	
65.	(VP-01) Zinc Vaporizers	109.1	
	TOTAL	1,790.7	(1975 dollars)
		x 1.4	inflation
		2,507.0	(1980 dollars)

TABLE 4.5-9

PRODUCTION LABOR COST FOR BCL PROCESS-CASE B

	Section	Labor Man-Hr/Kg Si	Labor Cost $/Man-Hr	Cost $/Kg Si
1.	Purification	0.01402	6.90	0.0968
2.	Deposition	0.01402	6.90	0.0968
3.	Electrolysis	0.02103	6.90	0.1451
4.	Waste Treatment	0.00701	6.90	0.0484
5.	Product Handling	0.00701	6.90	0.0484
			TOTAL	0.4355 (1975 dollars)
				x 1.4 inflation
				0.6097 (1980 dollars)

Note: Costs are 1975 Dollars

TABLE 4.5-10

ESTIMATION OF PLANT INVESTMENT FOR BCL PROCESS-CASE B

			Investment $1000	
1.		DIRECT PLANT INVESTMENT COSTS		
	1.	Major Process Equipment Cost	1,790.7	
	2.	Installation of Major Process Equipment	770.0	
	3.	Process Piping, Installed	1,325.1	
	4.	Instrumentation, Installed	340.2	
	5.	Electrical, Installed	179.1	
	6.	Process Buildings, Installed	179.1	
1a.		SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	4,584.2	
2.		OTHER DIRECT PLANT INVESTMENT COSTS		
	1.	Utilities, Installed	859.5	
	2.	General Service, Site Development, Fire Protection, etc.	214.9	
	3.	General Buildings, Offices, Shops, etc.	250.7	
	4.	Receiving, Shipping Facilities	376.1	
2a.		SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	1,701.2	
3.		TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	6,285.4	
4.		INDIRECT PLANT INVESTMENT COSTS		
	1.	Engineering, Overhead, etc.	984.9	
	2.	Normal Cont. for Floods, Strikes, etc.	1,271.4	
4a.		TOTAL INDIRECT PLANT INVESTMENT COST	2,256.3	
5.		TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	8,541.6	
6.		OVERALL CONTINGENCY, % of 5	1,708.3	
7.		FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	10,250.0	(1975 dollars)
			x 1.4	inflation
			14,350.0	(1980 dollars)

TABLE 4.5-11

ESTIMATION OF TOTAL PRODUCT COST FOR BCL PROCESS - CASE 3

	$/KG of Si
1. Direct Manufacturing Cost (Direct Charges)	
1. Raw Materials	2.091
2. Direct Operating Labor	0.436
3. Utilities	1.083
4. Supervision and Clerical	0.065
5. Maintenance and Repairs	1.025
6. Operating Supplies	0.205
7. Laboratory Charge	0.065
2. Indirect Manufacturing Cost (Fixed Charges)	
1. Depreciation	1.025
2. Local Taxes	0.205
3. Insurance	0.103
3. Plant Overhead	0.608
4. By-Product Credit	------
4a. Total Manufacturing Cost, 1 + 2 + 3 + 4	6.881
5. General Expenses	
1. Administration	0.413
2. Distribution and Sales	0.413
3. Research and Development	0.206
6. Total Cost of Product, 4a + 5	7.913 (1975 dollars)
	x 1.4 inflation
	11.078 (1980 dollars)

4.6 DCS Process (Dichlorosilane)

The economic analysis activity involves a cost analysis of the DCS process - Case A to produce dichlorosilane which is involved in the Hemlock Semiconductor Corporation program for polysilicon.

The cost analysis for the particular technology is based on process design results, such as requirements for raw materials and major process equipment necessary to produce the product from the chemical engineering analysis activity. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in the analysis of polysilicon production from dichlorosilane.

The cost analysis result for the DCS process (Case A) are presented in Table 4.6-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of $1.29 per kg of DCS (1980 dollars). This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses.

The product cost represents all cost associated with producing 1 kg of DCS. On top of these costs a producing company will include some profit. The sales price of the product silicon will actually be the sum of the product cost and a profit for the company. The profit is usually measured in terms of rate of return on the capital investment that the company spent in going into the DCS business. Two profitability methods which are commonly used are the return on original investment (per cent ROI) and discounted cash flow rate of return (per cent DCF).

The cost and profitability analysis summary for this process are presented in Table 4.6-2. The sales price of dichlorosilane at various rates of return for both profitability methods (per cent ROI and DCF) is shown in the lower half of the table. The results indicate a sales price of $1.47 per kg (1980 dollars) at 15 per cent DCF rate of return on investment.

These cost and profitability results for the DCS process will help the analysis of polysilicon production from dichlorosilane.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

- Preliminary Economic Analysis Activities...Table 4.6-3
- Process Design Inputs.......................Table 4.6-4
- Base Case Conditions........................Table 4.6-5
- Raw Material Cost...........................Table 4.6-6
- Utilitiy Cost...............................Table 4.6-7
- Major Process Equipment Cost................Table 4.6-8
- Production Labor Cost.......................Table 4.6-9
- Plant Investment............................Table 4.6-10
- Total Product Cost..........................Table 4.6-11

The economic analysis provides detailed cost data for raw materials, utilities, labor and major process equipment which are necessary for polysilicon production.

TABLE 4.6-1

ESTIMATION OF PRODUCT COST FOR DCS PROCESS

		Cost $/Kg of DCS (1975 dollars)	Cost $/Kg of DCS (1980 dollars)
1.	Direct Manufacturing Cost (Direct Costs)...... Raw Materials Direct Operating Labor Utilities Supervision and Clerical Maintenance and Repairs Operating Supplies Laboratory Charge	0.6935	0.9709
2.	Indirect Manufactuing Cost (Fixed Cost)....... Depreciation Local Taxes Insurance	0.0735	0.1029
3.	Plant Overhead................................	0.0355	0.0497
4.	General Expenses............................. Administration Distribution and Sales Research and Development	0.1205	0.1687
5.	Product Cost Without Profit..................	0.9230	1.2922

TABLE 4.6-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR DCS PROCESS

1. Process.................................... DCS process
2. Plant Size...................................9,780 metric tons/year
3. Plant Product................................ dichlorosilane
4. Product Form................................. liquid
5. Plant Investment............................. 6.36×10^6 / 8.90×10^6 (1975 dollars) (1980 dollars)

Fixed Capital		5.53 Mega	7.74 Mega
Working Capital (15%)	Total	0.83 Mega 6.36 Mega	1.16 Mega 8.90 Mega
		(1975 dollars)	(1980 dollars)

6. Return on Original Investment, after taxes (%ROI)

	Sales Price $/Kg of DCS (1975 dollars)	Sales Price $/Kg of DCS (1980 dollars)
0% ROI...............	0.92	1.29
5% ROI...............	0.98	1.38
10% ROI...............	1.04	1.46
15% ROI...............	1.10	1.55
20% ROI...............	1.16	1.63
25% ROI...............	1.22	1.71
30% ROI..............	1.28	1.80
40% ROI..............	1.40	1.97

7. Discounted Cash Flow Rate of Return, after taxes (% DCF)

	Sales Price $/Kg of DCS (1975 dollars)	Sales Price $/Kg of DCS (1980 dollars)
0% DCF..............	0.92	1.29
5% DCF..............	0.96	1.35
10% DCF..............	1.00	1.41
15% DCF..............	1.05	1.47
20% DCF..............	1.10	1.54
25% DCF..............	1.15	1.61
30% DCF..............	1.20	1.69
40% DCF..............	1.32	1.84

Based on 10 year project life and 10 year straight line depreciation.

TABLE 4.6-3

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR DCS PROCESS

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	●
1. Base Year for Costs	●
2. Appropriate Indices for Costs	●
3. Additional	●
3. Raw Material Costs	●
1. Base Cost/Lb of Material	●
2. Material Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
4. Utility Costs	●
1. Base Cost for Each Utility	●
2. Utility Cost/Kg of Silicon	●
3. Total Cost/Kg of Silicon	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●

Prel. Process Economic Activity	Status
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost/Kg Silicon Per Area	●
3. Total Cost/Kg Silicon	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○ Plan
◐ In Progress
● Complete

TABLE 4.6-4

PROCESS DESIGN INPUTS FOR DCS PROCESS

1. Raw Material Requirements
   -silicon tetrachloride, zinc, lime, argon and nitrogen
   -see table for "Raw Material Cost"

2. Utility
   -electricity, steam, cooling water and process water
   -see table for "Utility Cost"

3. Equipment List
   -process vessels, heat exchangers, reactors, etc.
   -see table for "Major Process Equipment Cost"

4. Labor Requirements
   -production labor for purification, deposition, electrolysis, etc.
   -see table for "Production Labor Cost"

TABLE 4.6-5
BASE CASE CONDITION FOR DCS 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

3. Raw Material Cost

   - Chemical Marketing Reporter
   - January 1975 Value
   - Raw Material Cost Index for Industrial Chemicals
   - 1975 Cost Index Value = 206.9 (Wholesale Price Index, Producer Price Index)

4. Labor Cost

   - Average for Chemical Petroleum, Coal and Allied Industries (1975)
   - Skilled $6.90/hr

5. Update to 1980

   - historically cited 1975 dollars (LSA project)
   - DOE decision to change to 1980 dollars (JPL, 6/22/79)
   - reports to reflect both 1975 and 1980 dollars (JPL, 6/22/79)
   - inflation factor of 1.4 to be used (JPL, 6/22/79)

TABLE 4.6-6

RAW MATERIAL COST FOR DCS PROCESS

	Raw Material	Requirement lb/kg of DCS	$/lb of material	Cost $/kg of DCS
1.	M.G. Silicon (Si)	0.348	0.535	0.1862
2.	Silicon Tetrachloride ($SiCl_4$, make-up)	1.987	0.135	0.2682
3.	Liquid Hydrogen	0.048	1.84	0.0883
4.	Copper Catalyst (Cu)	0.005	0.922	0.0046
5.	Hydrate Lime ($Ca(OH)_2$)	0.236	0.015	0.0036
			TOTAL	0.5509 (1975 dollars)
				x 1.4 inflation
				0.7713 (1980 dollars)

TABLE 4.6-7

UTILITY COST FOR DCS PROCESS

	Utility	Requirement/kg of DCS	Cost of Utility	Cost $/kg of DCS
1.	Electricity	0.337 KW HR	0.0324$/kw hr	0.01092
2.	Steam	12.81 lb	1.35$/Mlb	0.01730
3.	Cooling water	56.51 gal	0.09$/M gal	0.00509
4.	Process water	0.301 gal	0.405$/M gal	0.00012
5.	Fuel Oil	0.00473 MM Btu	1.40$/MM Btu	0.00662
			TOTAL	0.04005 (1975 dollars)
				x 1.4 inflation
				0.05607 (1980 dollars)

TABLE 4.6-5

PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR DCS PROCESS

	Equipment	Purchased Cost, $1000
1.	R-01 Hydrochlorination Reactor	81.9
2.	R-02 TCS Redistribution Reactor	14.0
3.	R-03 Wast Neutralizer	15.7
4.	R-04 Waste Combustor	8.0
5.	D-01 Crude TCS Stripping Column	5.40
6.	D-02 TCS/STC Distillation Column	40.41
7.	D-03 DCS/TCS Distillation Column	94.43
8.	D-04 DCS Distillation Column	41.22
9.	B-01 Silicon Storage Bin with Feed Lock	18.0
10.	T-01 Residue Settling Tank	55.8
11.	T-02 Residue Withdraw Tank	4.0
12.	T-03 Hydrogen Separation Tank	7.9
13.	T-04 Crude TCS Storage Tank	7.5
14.	T-05 TCS Stripper Reflux Drum	0.8
15.	T-06 TCS/STC Distillation Reflux Drum	4.5

TABLE 4.6-8 (continued)

16.	T-07 STC Storage Tank	13.8
17.	T-08 DCS/TCS Distillation Reflux Drum	6.9
18.	T-09 DCS Distillation Reflux Drum	1.2
19.	T-10 DCS Storage Tank (3)	23.9 ea.
20.	T-11 Flue Gas Separation Tank	0.8
21.	T-12 Lime Solution Preparation Tank	0.9
22.	T-13 Waste Filtrate Storage Tank	0.0
23.	H-01 Crude TCS Condenser	35.7
24.	H-02 H_2 Gas Preheater	27.2
25.	H-03 STC Vaporizer	54.5
26.	H-04 Stripper Condenser	2.0
27.	H-05 Stripper Reboiler	3.6
28.	H-06 TCS Condenser	53.4
29.	H-07 TCS/STC Reboiler	17.7
30.	H-08 STC Heat Exchanger	23.4
31.	H-09 DCS Condenser	13.4
32.	H-10 DCS/TCS Reboiler	14.7
33.	H-11 TCS Cooler	7.2
34.	H-12 DCS Distillation Overhead Condenser	1.6
35.	H-13 DCS Distillation	0.6
36.	H-14 Waste Stream Cooler	6.1
37.	H-15 STC Superheater	26.7
38.	H-16 H_2 Compressor Intercooler	3.6

TABLE 4.6-8 (continued)

39.	C-01A Hydrogen Feed Compressor, First-stage	26.0	
40.	C-01B Hydrogen Feed Compressor, Second-stage	26.0	
41.	C-02 Hydrogen Circulation Compressor	16.4	
42.	P-01 Feed Tank Blower	8.0	
43.	P-02 Settling Tank Circulation Pump	2.4	
44.	P-04 TCS Reflux Pump	2.7	
45.	P-05 STC Feed Pump	2.7	
46.	P-06 DCS Reflux Pump	1.0	
47.	P-08 DCS Purification Discharge Pump	0.3	
48.	P-09 DCS Pump	6.9	
49	P-10 Waste Solution Pump	0.5	
50.	P-11 Lime Solution Circulation Pump	0.5	
51.	P-12 Fresh Lime Solution Pump	0.4	
52.	F-01 Silicon Dust Filter	1.6	
53.	F-03 Waste Slurry Filter	5.0	
54.	S-01 Silicon Feed Cyclone	1.4	
55.	E-01 Quench Contact Ejector	1.3	
56.	E-02 Flue Gas Ejector	1.3	
		891.6	(1975 dollars)
		x 1.4	inflation
		1,248.2	(1980 dollars)

TABLE 4.6-9

PRODUCTION LABOR COST FOR DCS PROCESS

	Section	Labor man-hr/Kg DCS	Labor $/man-hr	Cost $/Kg DCS
1.	Hydrochlorination	0.001294	6.90	0.008929
2.	Purification/Redistribution	0.001941	6.90	0.013393
3.	Waste Treatment	0.000647	6.90	0.004464
				0.02679 (1975 dollars)
				x 1.4 inflation
				0.03751 (1980 dollars)

TABLE 4.6-10

ESTIMATION OF PLANT INVESTMENT FOR DCS PROCESS

		Investment $1000	
1.	DIRECT PLANT INVESTMENT COSTS		
	1. Major Process Equipment Cost	891.6	
	2. Installation of Major Process Equipment	383.4	
	3 Process Piping, Installed	659.8	
	4. Instrumentation, Installed	169.4	
	5. Electrical, Installed	89.2	
	6. Process Buildings, Installed	89.2	
1a.	SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	2,282.5	
2.	OTHER DIRECT PLANT INVESTMENT COSTS		
	1. Utilities, Installed	428.0	
	2. General Services, Site Development, Fire Protection, etc.	107.0	
	3. General Buildings, Offices, Shops, etc.	124.8	
	4. Receiving, Shipping Facilities	187.2	
2a.	SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	847.0	
3.	TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	3,129.5	
4.	INDIRECT PLANT INVESTMENT COSTS		
	1. Engineering, Overhead, etc.	490.4	
	2. Normal Cont. for Floods, Strikes, etc.	633.0	
4a.	TOTAL INDIRECT PLANT INVESTMENT COST	1,123.4	
5.	TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	4,252.9	
6.	OVERALL CONTINGENCY, % OF 5	1,275.9	
7.	FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	5,528.8	(1975 dolla
		x 1.4	inflation
8.	WORKING CAPITAL INVESTMENT FOR PLANT, % OF 6	7,740.3	(1980 doll
9.	TOTAL PLANT INVESTMENT, 7 + 8		

TABLE 4.6-11

ESTIMATION OF TOTAL PRODUCT COST FOR DCS PROCESS

		$/KG of DCS	
1.	Direct Manufacturing Cost (Direct Charges)		
	1. Raw Materials - from prel. design	0.5519	
	2. Direct Operating Labor - from prel. design	0.0268	
	3. Utilities - from prel. design	0.0400	
	4. Supervision and Clerical	0.0040	
	5. Maintenance and Repairs	0.0565	
	6. Operating Supplies	0.0113	
	7. Laboratory Charge	0.0040	
	8. Patents and Royalties		
2.	Indirect Manufacturing Cost (Fixed Charges)		
	1. Depreciation	0.0565	
	2. Local Taxes	0.0113	
	3. Insurance	0.0057	
3.	Plant Overhead	0.0355	
4.	By-Product Credit - from prel. design		
4a.	Total Manufacturing Cost, 1 + 2 + 3 + 4	0.8026	
5.	General Expenses		
	1. Administration	0.0482	
	2. Distribution and Sales	0.0482	
	3. Research and Development	0.0241	
6.	Total Cost of Product, 4a + 5	0.9230	(1975 dollars)
		x 1.4	inflation
		1.2922	(1980 dollars)

5. SUMMARY - CONCLUSIONS

The following summary-conclusions are made as a result of analyses conducted for new technologies and processes being developed for the production of lower cost silicon for solar cells:

1. Analyses of process system properties are important for chemical materials involved in the several processes under consideration for semiconductor and solar cell grade silicon production. Major physical, thermodynamic and transport property data are reported for the following silicon source and processing chemical materials

   - Silane
   - Silicon Tetrachloride
   - Trichlorosilane
   - Dichlorosilane
   - Silicon Tetrafluoride
   - Silicon

   The property data are reported for critical temperature, critical pressure, critical volume, vapor pressure, heat of vaporization, heat capacity, density, surface tension, viscosity, thermal conductivity, heat of formation and Gibb's free energy of formation. The reported property data are presented as a function of temperature to permit rapid usage in research, development and production engineering.

2. Chemical engineering analyses involving the preliminary process design of a plant (1000MT/yr capacity) to produce silicon via the techology under consideration were accomplished for the following processes:

   - UCC Silane Process for Silicon
   - BCL Process for Silicon - Case A
   - BCL Process for Silicon - Case B
   - Conventional Polysilicon Process (Siemen's Technology)
   - SiI_4 Decomposition Process
   - DCS Process (Dichlorosilane)

   Major activities in the chemical engineering analyses included base case conditions, reaction chemistry, process flowsheet, material balance, energy balance, property data, equipment design, major equipment list, production labor and forward for economic analysis. The process design package provided detailed data for raw materials, utilities, major process equipment and production labor requirements necessary for polysilicon production in each process.

3. Economic analyses were accomplished for the following processes under consideration for the production of silicon:

- UCC Silane Process for Silicon
- BCL Process for Silicon - Case A
- BCL Process for Silicon - Case B
- Conventional Polysilicon Process (Siemens Technology)
- SiI_4 Decomposition Process
- DCS Process (Dichlorosilane)

Primary activities in the economic analyses involved process design inputs, base case conditions, raw material costs utility costs, major process equipment costs and production labor costs in the estimation of plant investment and total product cost.

4. The cost analysis results for producing silicon by the UCC silane process (Union Carbide Corporation) are presented including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon) The results indicate a total product cost without profit of $6.90 (1975 dollars) and $9.66 (1980 dollars) per kg. For profitability analysis, the results indicate a sales price of $13 per kg of silicon (1980 dollars) at 15 per cent DCF (discounted cash flow) rate of return on investment.

These cost and profitability results for the UCC silane process indicate that this new technology for producing polysilicon shows good promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

5. The cost analysis results for producing silicon by the BCL process - Case A (Battelle Columbus Laboratories) are presented including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The results indicate a total product cost without profit of $8.63 (1975 dollars) and $12.08 (1980 dollars) per kg. The profitability analysis results disclose a sales price of $13.28 per kg of silicon (1980 dollars) at 5 per cent DCF (discounted cash flow) rate of return on investment after taxes.

These cost and profitability results for the BCL process - Case A indicate that this new technology for producing polysilicon shows promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells. In Case A, the process involves two deposition reactors and six electrolysis cells.

6. The cost analysis results for producing silicon by the BCL process - Case B (Battelle Columbus Laboratories) are presented including costs for raw materials, labor, utilities and other items composing the product cost

(total cost of producing silicon). The results give a total product cost without profit of $7.91 (1975 dollars) and $11.07 (1980 dollars) per kg. For profitability, the analysis indicates a sales price of $13.14 per kg of silicon (1980 dollars) at 10 per cent DCF (discounted cash flow) rate of return on investment.

These cost and profitability results for the BCL process - Case B indicate that this new technology for producing polysilicon shows promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells, In Case B, the process contains one deposition reactor and two electrolysis cells.

7. For the conventional polysilicon process, the cost analysis is based on a poly plant constructed in the 1960's (1965 or earlier) since several existing plants producing semiconductor grade polysilicon in the United States were constructed in the 1960's. The operating costs for the plant are applicable to the time period of interest (such as 1975 and 1980).

The cost analysis results for producing silicon by the conventional Siemens process are presented including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The results disclose total product cost without profit of $35.52 - 41.29 (1975 dollars) and $49.73 - 57.81 (1980 dollars) per kg. The range for product cost reflects low and high electrical costs (1.5-3¢/kw hr for 1975 and 2.1-4.2¢/kw hr for 1980).

The average product cost without profit is estimated at $38.41 (1975 dollars) and $53.77 (1980 dollars) per kg for the conventional polysilicon process. This average product costs corresponds to intermediate electrical costs (2.25¢/kw hr for 1975 and 3.15¢/kw hr for 1980). These costs results for the conventional polysilicon process indicate that this Siemens technology using trichlorosilane for producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

8. The cost analysis results for producing silicon by the SiI_4 decomposition process are presented including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The results give a total product cost without profit of $44.64 (1975 dollars) and $62.50 (1980 dollars) per kg. The profitability results indicate a sales price of $71.48 per kg of silicon (1980 dollars) at 5 per cent DCF (discounted cash flow) rate of return on investment.

These cost and profitability results for the SiI_4 decomposition process indicate that this new technology for producing polysilicon does not show promise for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

9. Using a hot-wire technique, experimental gas phase thermal conductivity values were determined between 25°C and 350°C for silicon source materials such as silane and halogenated silanes. The accuracy of the values were shown to be ±2% by determining values for argon and hydrogen, compounds whose thermal conductivity values have been previously determined.

10. Experimental gas phase viscosity values were determined for the halogenated silanes; dichlorosilane, trichlorosilane and tetrafluorosilane. The values were determined in the temperature range 40°C to 200°C using a transpiration method. Nitrogen, a compound for which viscosity values are known, was used to calibrate the apparatus. The calibration studies showed that the values obtained were accurate to ±2% throughout the temperature range.

11. Studies were conducted to develop an efficient method for the generation of SiF_4 from hexafluorosilicic acid, a readily available by-product of the phosphate fertilizer industry. This included investigation of such parameters as conditions for precipitation of SiF_4 precursors (Na_2SiF_6 and $BaSiF_6$), temperature for thermal decomposition of the salts, heating time required and optimum flow rates. Precipitation of the salts, Na_2SiF_6 or $BaSiF_6$, with NaCl, NaF, $BaCl_2$, or BaF_2 followed by thermal decomposition at temperatures above 500°C proved to be an efficient method for the generation of SiF_4.

A1. ADDITIONAL CHEMICAL ENGINEERING ANALYSIS

A1.1 Silane Process - Case A

The chemical engineering analysis activity of Silane Process - Case A (Regular Process Storage) involves a preliminary process design of a plant to product silane for silicon.

The Silane Process- Case A involves several processing operations of hydrogenation, distillation, redistribution reaction, stripping and absorption. The process flowsheet is shown in Figure A1.1-1. This flowsheet was received from Union Carbide.

A summation of the salient features of Case A is shown below:

CASE A

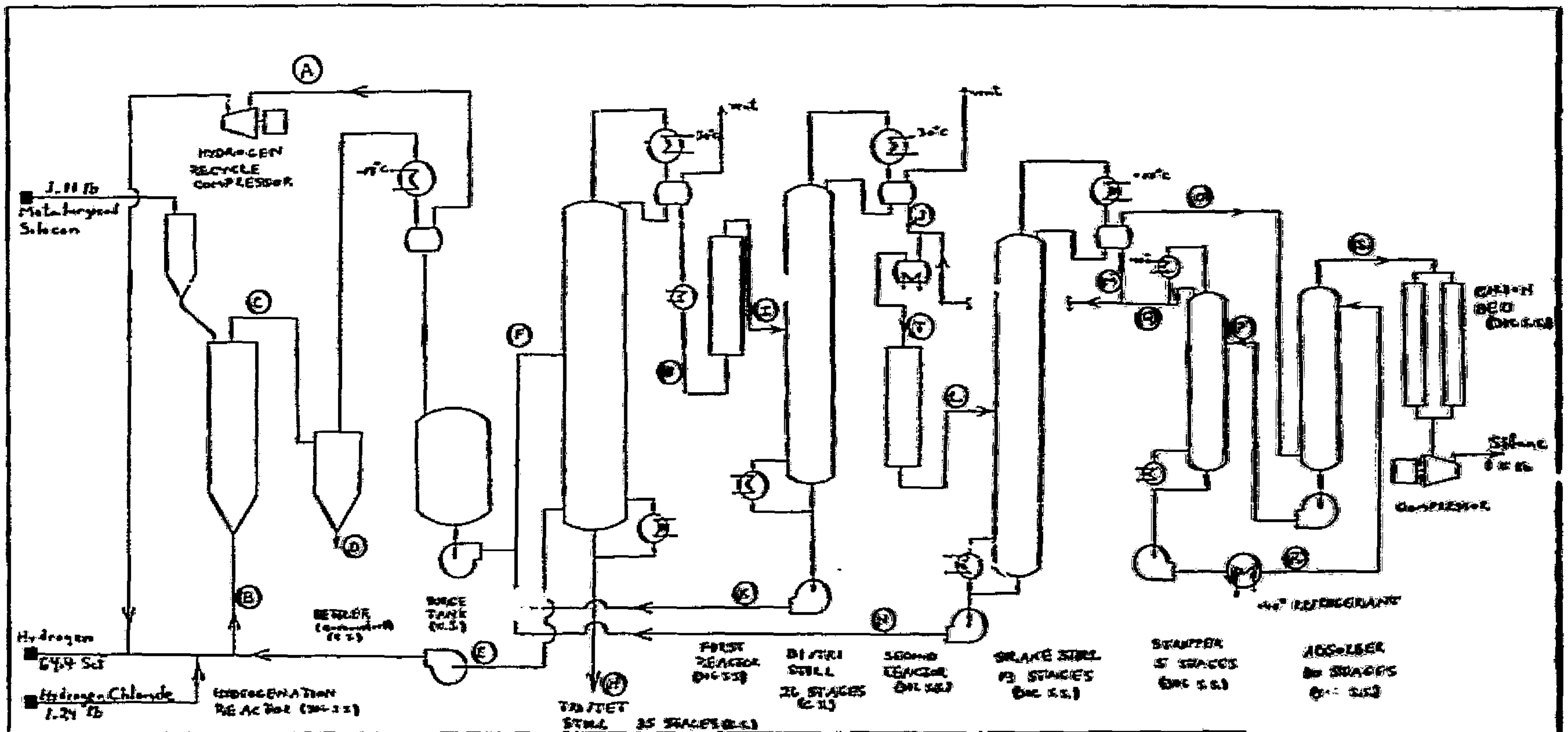
Process	Silane (Union Carbide)
Plant Size	1270 MT/year of Silane
Process Flowsheet	Original received from Union Carbide
Process Chemistry and Equilibrium	From Union Carbide
Intermediate Product Storage Considerations	Regular
Major Process Equipment	76 pieces of process equipment

The detailed status sheet is shown in Table A1.1-1, and is representative of the various subitems that make up the preliminary design activity. The results from the preliminary process design are presented in a tabular format similar to previous design results for alternate processes to produce silicon. Note that in this process results are per pound of silane versus other processes represented as per kilogram of silicon. The silane plant size assumes a 90% conversion of silane to silicon.

The guide to the tables for Case A is given below:

Base Case Conditions	Table A1.1-2
Reaction Chemistry	Table A1.1-3
Raw Material Requirement	Table A1.1-4
Utility Requirements	Table A1.1-5
Major Process Equipment	Table A1.1-6
Production Labor Requirements	Table A1.1-7

CASE A



Ref. Point	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
Temp., °C	-17	550	550	110	134		80	[illegible]	80	25	75	20	-5	25	-5	-5	-6	-40	-90	80		
Press., psig	50	50	45	35	50	60	50	50	50	50	50	45	45	50	45	35	35	45	45	45		
Flow, lb/hr	6.6	139	140	.6	131	268	136	1.3	136	.02	135	24.7	9.2	9.0	3.3	3.35	6.9	1.6	1.05	26.7		
H_2, mole %	99.7	97.5	46.7	-	-	-	-	-	-								-	-	-			
$SiCl_4$, mole %	2.6	73.2	93.3	80	97.0	92.8	-	99.5	86.5		12.9					36.9	-	97.6	.2			
$HSiCl_3$, mole %	1.7	.3	10.3	20	1.0	57.2	97.0	.5	73	1	87.2	99	4.4	98.3		-	-		-	2.5		
H_2SiCl_2, mole %	-	-	-		-	-	1.0		10	99		35	67.8	1.5	85.1	38.8	99.3		-	59.2		
H_3SiCl, mole %	-	-	-		-	-			0.5			11	22.9		16.8	21	98.6	0.5	.7	6.2		
SiH_4, mole %	-	-	-		-	-			-			2.0	12.4		22.2	5.4	3.1		99.1	5.1		
HCl, mole %		1.1	-		-	·																

CHEMICALS & PLASTICS

Silicon to Silane [illegible]

C-1097-2

Figure A1.1-1 Process Flow Sheet for Silane Process-Case A
(Provided by Union Carbide)

CASE A

TABLE A1.1-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR SILANE PROCESS - CASE A

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

○ Plan
◐ In Progress
● Complete

CASE A

TABLE A1.1-2

BASE CASE CONDITIONS FOR SILANE PROCESS - CASE A

1. Plant Size:
   - Allow for 10% losses of silane in production of silicon
   - 1270 metric tons/year of silane
   - Solar cell grade silicon

2. Hydrogenation Reaction
   - Metallurgical grade silicon, hydrogen, to produce trichlorosilane (TCS) make-up hydrogen chloride used and recycle silicon tetrachloride (TET)
   - Copper catalyzed
   - Fluidized bed
   - 550°C, 50 PSIG
   - 15.8% conversion of $SiCl_4$ (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 30 PSIG, 80°C.
   - Conversion a function of inlet concentration per Figure IIA-2 (Union Carbide equilibrium)
   - Conversion from pure TCS feed is about 10% to DCS (example)
4. DCS Redistribution Reaction
   - DCS produces 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-1.1 (Union Carbide equilibrium)
   - Conversion from pure DCS feed is about 14% to Silane (example)
5. Recycles
   - Unreacted chlorosilanes separated by distillation and recycled

6. Silane Purification
   - Chlorosilanes removed by absorption in -40°C $SiCl_4$ (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)

CASE A

TABLE A1.1-3

REACTION CHEMISTRY FOR SILANE PROCESS - CASE A

1. Hydrogenation Reaction

$$3\ SiCl_4 + Si + 2H_2 \rightleftarrows 4SiHCl_3$$

2. Trichlorosilane Redistribution Reaction

$$2\ SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4$$

3. Dichlorosilane Redistribution Reaction

$$3\ SiH_2Cl_2 \xrightarrow{\text{Distillation}} 2SiHCl_3 + SiH_4$$

Note

1. Reaction 1 Product contains H_2, $SiCl_4$, $SiHCl_3$, SiH_2Cl_2 (trace), other trace chlorides
2. Reaction 2 Product contains $SiHCl_3$, $SiCl_4$, SiH_2Cl_2, SiH_3Cl
3. Reaction 3 Product contains SiH_2Cl_2, $SiHCl_3$, $SiCl_4$, SiH_3Cl, SiH_4

CASE A

TABLE A1.1-4

RAW MATERIAL REQUIREMENTS FOR SILANE PROCESS - CASE A

	Raw Material	Requirement lb/lb of Silane
1.	Anhydrous HCl	1.239
2.	Hydrogen	.362
3.	Caustic (50%)	2.448
4.	M.G. Silicon	1.11

CASE A

TABLE A1.1-5

UTILITY REQUIREMENTS FOR SILANE PROCESS - CASE A

Utility/Function	Requirements/lb of Silane Product	
1. Electricity		.253 KW-HR
1. All pump and compressor motors (24)	(.253)	
2. Steam 250 Psia		190.34 lbs
1. #1 Distillation Column Preheater	(6.96)	
2. #1 Distillation Column Reboiler	(81.18)	
3. #2 Distillation Column Reboiler	(91.77)	
4. #2 Redistribution Reactor Preheater	(3.0)	
5. #3 Distillation Column Preheater	(3.62)	
6. #3 Distillation Column Reboiler	(3.29)	
7. #4 Distillation Column Reboiler	(.41)	
8. Waste Treatment	(.11)	
3. Cooling Water (10-120°F)		168.12 gallons
1. #1 Distillation Column Condenser	(146.12)	
2. #2 Distillation Column Condenser	(22.00)	
4. Process Water (90°F)		8.22 gallons
1. Waste Treatment	(8.22)	
5. Refrigerant (23°F)		27.1 BTU
1. #4 Distillation Column Feed Tank	(27.1)	
6. Refrigerant (5°F)		79.1 BTU
1. #3 Distillation Column Overhead Receiver	(79.1)	
7. Refrigerant (-7°F)		26.4 BTU
1. #4 Distillation Column Overhead Receiver	(26.4)	
8. Refrigerant (-20°F)		2303.2 BTU
1. #3 Distillation Column Condenser	(2058.0)	
2. #4 Distillation Column Condenser	(245.2)	

CASE A

TABLE A1.1-5 (Continued)

9.	Refrigerant (-30°F)		30788.0 BTU
	1. TCS Reactor Recycle Gas Condenser	(30788.0)	
10.	Refrigerant (-40°F)		280.6 BTU
	1. #2 Redistribution Reactor Condensate Receiver	(192.2)	
	2. Silane Product Storage	(88.4)	
11.	Refrigerant (-50°F)		3503.2 BTU
	1. #2 Redistribution Reactor Gas Condensor	(2986.0)	
	2. Product Silane Condenser	(137.9)	
	3. Absorbent Cooler	(379.3)	
12.	High Temperature Heat Exchange Fluid		3.324×10^4 BTU
	1. TCS Reactor Recycle Gas Heater	(6.591×10^3)	
	2. HCl Vaporizer	(4.466×10^2)	
	3. Tet Vaporizer	(2.464×10^4)	
	4. Heat Nitrogen to Regenerate Char. Adsorbers	(70.95)	
	5. TCS Reactor	(1.491×10^3)	
13.	Nitrogen		5.54 SCF
	1. Regenerate Charcoal Adsorbers	(5.54)	

CASE A

TABLE A1.1-6

LIST OF MAJOR PROCESS EQUIPMENT FOR SILANE PROCESS – CASE A

Type	Function	Duty	Size	Materials of Construction
1. (T1) M.G. Silicon Storage Hopper	Raw Material Storage	2 weeks storage	1.363 x 10^4 gallons	CS
2. (T2) Hydrogen Storage Tank	Raw Material Storage	8 hours backup for pipeline failure	9.161 x 10^4 gallons 250 PSIA (spherical)	CS
3. (T3) Liquid HCl Storage Tank	Raw Material Storage	2 weeks storage	1.612 x 10^4 gallons 250 PSIA, -50°F (spherical)	Nickel Steel
4. (T4) Recycle TET Storage	For TCS Reactor Feed	2 days storage	1.985 x 10^5 gallons 65 PSIA	CS
5. (T5) TCS Reactor Off-Gas Flash Tank	Phase Separation		1 ft. diameter by 4 ft. long, 65 PSIA, 0°F 65 PSIA	CS
6. (T6) TCS/TET Storage	Feed Distillaton Column #1	2 Days hold-up	1.966 x 10^5 gallons 65 PTSA	CS
7. (T7) #1 Distillation Column Condensate Accumulator	Reflux feed; column Control	20 minutes hold-up	4.88 x 10^3 gallons 65 PSIA	CS
8. (T8) #1 Redistribution Reactor Feed Tank	Hold-up and feed Reactor	2 days hold-up	2.266 x 10^5 gallons 65 PSIA	CS
9. (T9) #1 Redistribution Reactor Product Tank	Hold-up and feed #2 Distillation Column	2 days hold-up	2.21 x 10^5 gallons 65 PSIA	CS

CASE A

TABLE A1.1-6 (continued)

10.	(T10)	#2 Distillation Column Condensate Accumulator	Reflux feed; column Control	20 minutes hold-up	746 gallons 65 PSIA	SS
11.	(T11)	#2 Redistribution Reactor Feed Tank	Hold-up and feed Reactor	2 days hold-up	1.891×10^4 gallons 65 PSIA	SS
12.	(T12)	#2 Redistribution Reactor Product Tank	Hold-up and feed #3 Distillation Column	2 days hold-up 6.8×10^4 BTU/hr	3.46×10^4 gallons -40°F, 60 PSIA	SS
13.	(T13)	#3 Distillation Column Condensate Accumulator	Reflux feed; phase Separation; column control	20 minutes hold-up	194 gallons 5°F, 60 PSIA	SS
14.	(T14)	#3 Distillation Column Condensate Tank	Hold-up and recycle feed to #2 Redistribution Reactor	2 days hold-up 2.81×10^4 BTU/hr	1.7×10^4 gallons 60 PSIA, 5°F	SS
15.	(T15)	#4 Distillation Column Feed Tank	Surge between absorber and distillation	2 days hold-up 9.63×10^3 BTU/hr	4.69×10^3 gallons 60 PSIA	SS
16.	(T16)	#4 Distillation Column Condensate Accumulator	Reflux feed; column control	20 minutes hold-up	16 gallons 50 PSIA,-7°F	SS
17.	(T17)	#4 Distillation Column Condensate Tank	Hold-up and recycle to #2 Redistribution Reactor	2 days hold-up 9.4×10^3 BTU/hr	2.55×10^3 gallons 50 PSIA, -7°F	SS
18.	(T18)	Waste Tank	Collect waste for Treatment and disposal	2 week storage	1.378×10^4 gallons 65 PSIA	CS
19.	(T19)	Absorber Feed Tank	Feed TET to absorber	2 days storage	2.44×10^3 gallons 50 PSIA	SS
20.	(T20)	Silane Storage	Final Product storage	1 week storage 3.14×10^4 BTU/hr	1.522×10^4 gallons -40°F, 250 PSIA	SS

TABLE A1.1-6 (continued)

21.	(T21)	Caustic Storage	Raw Material Storage	2 weeks storage	2.304 x 10^4 gallons	SS
22.	(H1)	TCS Reactor Recycle Gas Heater	Heat Recycle gas and Hydrogen to 550°C	2.342 x 10^6 BTU/hr	752 ft^2 65 PSIA	CS
23.	(H2)	HCl Vaporizer	Heat Reactant to 550°C	1.587 x 10^5 BTU/hr	34 ft^2 65 PSIA	CS
24.	(H3)	TET Vaporizer	Heat Reactant to 550°C	8.755 x 10^6 BTU/hr	2381 ft^2 65 PSIA	CS
25.	(H4)	TCS Reactor Recycle Condenser	Phase separation; Recycle hydrogen	1.094 x 10^7 BTU/hr	1882 ft^2 65 PSIA	CS/SS
26.	(H5)	#1 Distillation Column Preheater	Preheat distillation feed to bubble point	2.044 x 10^6 BTU/hr	164 ft^2 250 PSIA	CS
27.	(H6)	#1 Distillation Column Condenser	Provide Reflux to Column	1.296 x 10^7 BTU/hr	3189 ft^2 65 PSIA	CS
28.	(H7)	#1 Distillation Column Reboiler	Provide vapor to Column	2.382 x 10^7 BTU/hr	2818 ft^2 250 PSIA	CS
29.	(H8)	#2 Distillation Column Condenser	Provide Reflux to column	1.96 x 10^6 BTU/hr	956 ft^2 65 PSIA	CS/SS
30.	(H9)	#2 Distillation Column Reboiler	Provide Vapor to Column	2.693 x 10^7 BTU/hr	2514 ft^2 250 PSIA	CS
31.	(H10)	#2 Redistribution Reactor Feed Vaporizer	Vaporize Reactants for Reactor	8.81 x 10^5 BTU/hr	78 ft^2 250 PSIA	CS/SS
32.	(H11)	#2 Redistribution Reactor Product Condenser	Condense Vapor for hold-up storage	1.06 x 10^6 BTU/hr	306 ft^2 60 PSIA	CS/SS
33.	(H12)	#3 Distillation Column Preheater	Vaporize and preheat feed to column	1.06 x 10^6 BTU/hr	66 ft^2 250 PSIA	CS/SS

CASE A

TABLE A1.1-6 (continued)

34.	(H13)	#3 Distillation Column Condenser	Provide Column Reflux (Partial Condenser)	7.312×10^5 BTU/hr	593 ft^2 60 PSIA	CS/SS
35.	(H14)	#3 Distillation Column Reboiler	Provide Vapor to Column	9.64×10^5 BTU/hr	84 ft^2 250 PSIA	CS/SS
36.	(H15)	Silane Condenser	Condenser Final Product for storage	4.9×10^4 BTU/hr	53 ft^2 250 PSIA	CS/SS
37.	(H16)	#4 Distillation Column Condenser	Provide Reflux	8.71×10^4 BTU/hr	84 ft^2 50 PSIA	CS/SS
38.	(H17)	#4 Distillation Column Reboiler	Provide Vapor to Column	1.2×10^5 BTU/hr	13 ft^2 250 PSIA	CS/SS
39.	(H18)	Absorber Pre-cooler	Cool TET for absorption column	1.35×10^5 BTU/hr	35 ft^2 60 PSIA	CS/SS
40.	(H19)	Nitrogen Heater	Heat Nitrogen to regenerate Charcoal Adsorbers	2.52×10^4 BTU/hr	14.1 ft^2	CS
41.	(P1)	TCS Reactor Off Gas Recycle Compressor	Circulate Recycle Gas to Reactor	1.36×10^3 SCFM	26.5 Horsepower 75 PSIA Discharge	CS*
42.	(P2)	#1 Distillation Column Feed Pump	Feed Column	136.5 gpm	106 PSI; 14.5 BHP	CS*
43.	(P3)	#1 Distillation Column Overheads Pump	Provide Reflux and remove overhead product	244 gpm	92.3 PSI; 22.5 BHP	CS*
44.	(P4)	#1 Distillation Column Bottoms Pump	Remove Bottoms Product to TET storage tank	69 gpm	106 PSI; 7.3 BHP	CS*

CASE A

TABLE A1.1-6 (continued)

45.	(P5)	Process Water Feed Pump	Feed Process Water to Waste Treatment	48.6 gpm	82.5 PSI; 4 BHP	CS*
46.	(P6)	Caustic Feed Pump	Feed Raw Material to waste treatment	1 gpm	118 PSI; ¼ BHP	SS
47.	(P7)	#1 Redistribution Reactor Feed Pump	Feed TCS to Reactor	79 gpm	106 PSI; 8.4 BHP	SS
48.	(P8)	#2 Distillation Column Feed Pump	Feed TCS/DCS still	76.6 gpm	92.3 PSI; 7.1 BHP	SS
49.	(P9)	#2 Distillation Column Overheads Pump	Provide Reflux and Remove Overhead Product	37.3 gpm	92.3 PSI; 3.4 BHP	SS
50.	(P10)	#2 Distillation Column Bottoms Pump	Remove Bottoms Product to TCS/TET storage tank	66.7 gpm	106.3 PSI; 7.1 BPH	SS
51.	(P11)	#2 Redistribution Reactor Feed Pump	Feed DCS to Reactor	13.4 gpm	130 PSI; 1.7 BHP	SS
52.	(P12)	#3 Distillation Column Feed Pump	Feed Silane Still	12 gpm	87.3 PSI; 1 BHP	SS
53.	(P13)	#3 Distillation Column Overhead Pump	Provide Reflux; Remove Overhead Product	9.7 gpm	87.3 PSI; 1 BHP	SS
54.	(P14)	#3 Distillation Column Bottoms Pump	Remove Bottoms Product to TCS/TET Tank	5.2 gpm	106.3 PSI, ½ BHP	SS
55.	(P15)	#4 Distillation Feed Pump	Feed TET Stripper	1.6 gpm	77.3 PSI, ¼ BHP	SS

* Includes incremental higher cost for special purity requirements.

CASE A

TABLE A1.1-6 (continued)

56.	(P16)	#4 Distillation Column Overhead Pump	Provide Reflux, Remove Overhead Product	1 gpm	77.3 PSI; ¼ BHP	SS
57.	(P17)	#4 Distillation Column Bottoms Pump	Remove Bottoms Product to Absorber Feed Tank	1 gpm	91.3 PSI; ¼ BHP	SS
58.	(P18)	#4 Distillation Condensate Recycle Pump	Recycle Condensate back to #2 Redistribution Reactor	1 gpm	106.3 PSI; ¼ BHP	SS
59.	(P19)	Silane Product Compressor	Liquefy Silane for Storage	66 SCFM	250 PSIA Discharge 6.5 HP	SS
60.	(P20)	Waste Feed Pump	Distillation Wastes to Waste Treatment	1 gpm	76.3 PSI; ¼BHP	CS
61.	(P21)	TCS Reactor Feed Pump	Feed TET to Reactor	69 gpm	92.3 PSI; 6.4 BHP	CS*
62.	(P22)	#3 Distillation Condensate Recycle Pump	Recycle Condensate back to #2 Redistribution reactor	5.9 gpm	92.3 PSI; ½ BHP	SS
63.	(P23)	Waste Collection Pump	Distillation Wastes to Waste Tank	1 gpm	87.3 PSI; ¼ BHP	CS
64.	(P24)	Absorber Feed Pump	Feed Cold TET to Absorption Column	1 gpm	87.3 PSI; ¼ BHP	SS
65.	(C1)	#1 Distillation Column	Separate TET from TCS	95,220 lb/hr of feed	7.56 ft. diameter 100 ft. tall, 50 trays	CS

TABLE A1.1-6 (continued)

66.	(C2)	#2 Distillation Column	Separate TCS from DCS	48, 321 lb/hr of feed	10.6 ft. Diameter 136 ft. tall, 68 trays	CS
67.	(C3)	#3 Distillation Column	Separate Silane from other Chlorosilanes	7344 lb/hr of feed	2.01 ft. Diameter 29 ft. tall, 29 trays	SS
68.	(C4)	#4 Distillation Column	Strip TET for use in absorber	1007.7 lb/hr of feed	1.04 ft. Diameter 28.5 ft. tall, 38 trays	SS
69.	(C5)	Silane Absorber	Absorb Chlorosilane from Silane	819.3 lb/hr of vapor feed	0.823 ft. Diameter 12 ft. tall, 16 trays	SS
70.	(C6)	Charcoal Adsorber	Activated Carbon Adsorbtion of Silane to remove Trace Chlorosilane	366 lb/hr of vapor feed	1 ft. Diameter 7 ft. tall (2), 623 lbs of carbon	SS
71.	(R1)	TCS Fluidized Bed Reactor	Produces TCS from TET M.G.Silicon, and H_2		6.26 ft. in diameter 26.5 ft. tall, 481 tubes 1", 16' long	SS
72.	(R2)	#1 Redistribution Reactor	Redistribute TCS to DCS		2' Diameter by 15 ft. tall 1042 lbs catalyst	SS
73.	(R3)	#2 Redistribution Reactor	Redistribute DCS to Silane		2.34' Diameter by 35 ft.tall 1667.2 lbs catalyst	SS
74.	(A1)	Fines Separator	Remove Silicon Fines carried over with TCS Reactor Off-gas		Standard design 30" Diameter	SS
75.	(A2)	Waste Treatment	Discharge innocuous effluent		1 column for absorption + 1 heat exchanger to vaporize feed	SS
76.	(A3)	Hydrogen Flare	Dispose of Hydrogen from Waste Treatment		30 ft. stack 6" Diameter	CS

CASE A

TABLE A1.1-7

PRODUCTION LABOR REQUIREMENTS FOR SILANE PROCESS-CASE A

			Skilled Labor, Man Hours		Semiskilled Labor	
	Unit Operation	Type	Per Day	Per lb. Silane	Per Day	Per lb. Silane
1.	TCS Production	B	65	.0085		
2.	Hydrogen Recycle	C	18	.0023		
3.	Raw Material Vaporization	C	50	.0065		
4.	TCS Condensation	C	50	.0065		
5.	TCS/TET Separation	C	62	.0081		
6.	#1 Redistribution Reactor	C	49	.0064		
7.	DCS/TCS Separation	C	52	.0068		
8.	#2 Redistibuiton Reactor	C	32	.0042		
9.	Silane Distillation	C	32	.0042		
10.	Silane Absorption	C	28	.0036		
11.	Silane Purification (adsorption)	A	36	.0047		
12.	Silane compression	B	23	.003		
13.	Silane Condensation	B	23	.003		
14.	Materials Handling	A			48	.0063
15.	Waste Treatment	B	60	.0078		
16.	Silicon Fines Separation	A	15	.002		
	TOTAL		595	.0776	48	.0063

NOTES:

1. A Batch Process of Multiple Small Units
   B Average Process
   C Automated Process

2. Man hours/day Unit from Figure 4-6, Peters and Timmerhaus (7).

A1.2 Silane Process - Case B

The chemical engineering analysis of the Silane Process - Case B (Minimum Process Storage) involves a preliminary process design of a plant to produce silane for silicon.

The Silane Process - Case B involves several processing operations of hydrogenation distillation, redistribution, distillation, redistribution reaction, stripping and absorption. The flowsheet received from Union Carbide, upon which the design is based, is shown in Figure A1.2-1.

A summation of the important features of CASE B is presented in the following table:

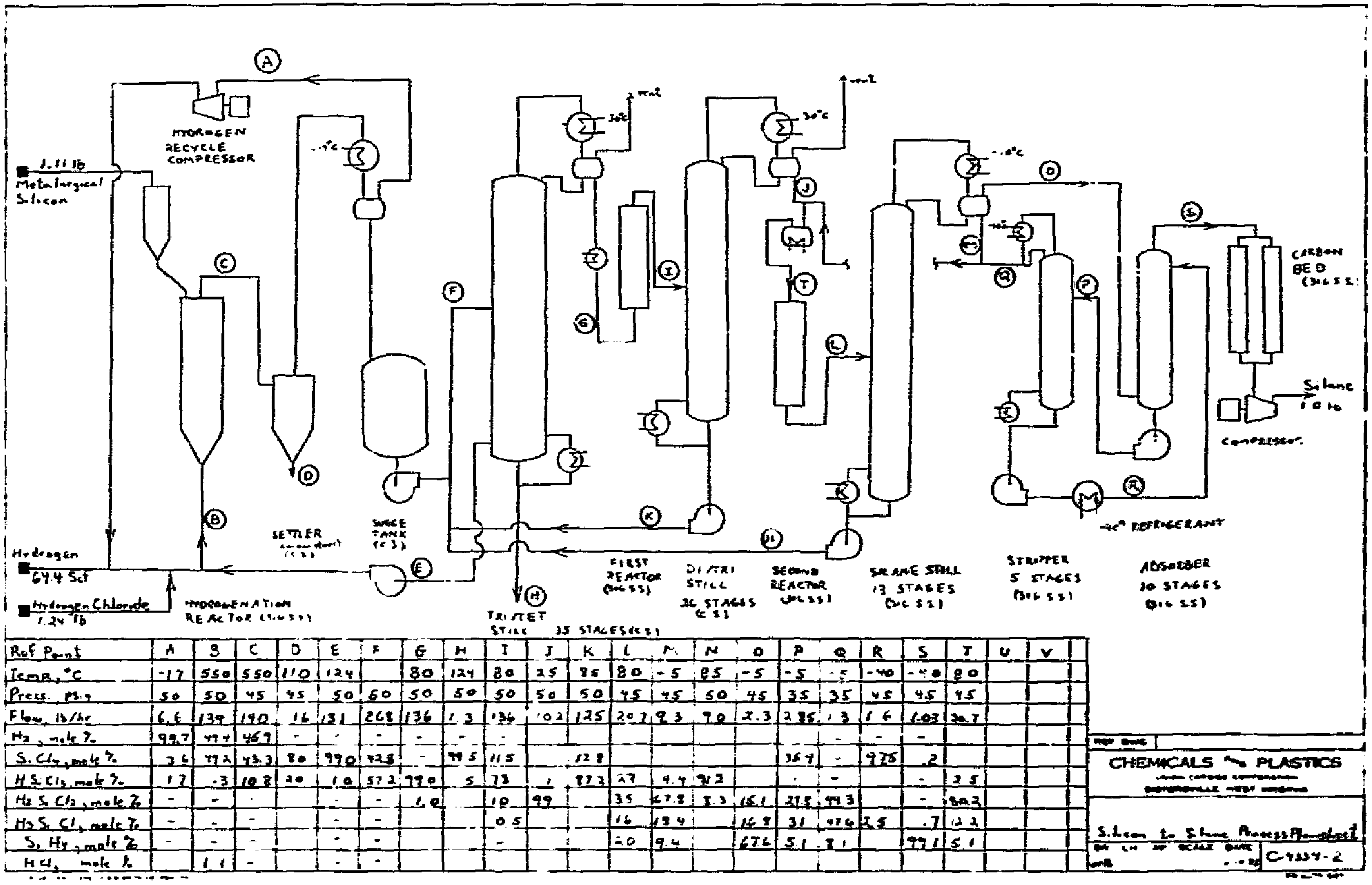
CASE B

Process	Silane (Union Carbide)
Plant Size	1270 MT/year of Silane
Process Flow Sheet	Original Received from Union Carbide
Process Chemistry & Equilibrium	From Union Carbide
Intermediate Product Storage Considerations	Minimum
Major Process Equipment	58 pieces of Process Equipment

The results from the preliminary process design (CASE B) are summarized in a tabular format parallel to those representing Case A. These tables are represented by the following guide to enable the reader to quickly locate items of interest.

Base Case Conditions	Table A1.2-2
Reaction Chemistry	Table A1.2-3
Raw Material Requirement	Table A1.2-4
Utility Requirements	Table A1.2-5
Major Process Equipment	Table A1.2-6
Production Labor Requirements	Table A1.2-7

CASE B



Ref Point	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
Temp., °C	-17	550	550	110	124		80	124	80	25	85	80	-5	85	-5	-5	-5	-40	-40	80		
Press. psig	50	50	45	45	50	60	50	50	50	50	50	45	45	50	45	35	35	45	45	45		
Flow, lb/hr	6.6	139	140	16	131	268	136	1.3	136	.02	125	20.7	9.3	90	2.3	2.85	.13	1.6	1.03	30.7		
H_2, mole %	99.7	47.4	46.9	-	-	-	-	-	-								-	-	-			
$SiCl_4$, mole %	3.6	47.2	43.3	80	99.0	42.8	-	99.5	11.5		12.8					36.9	-	97.5	.2			
$HSiCl_3$, mole %	1.7	.3	10.8	20	1.0	57.2	99.0	.5	73	.1	87.2	27	4.4	91.2		-	-		-	2.5		
H_2SiCl_2, mole %	-	-	-		-	-	1.0		10	99		35	67.8	8.8	16.1	21.5	99.3		-	80.2		
H_3SiCl, mole %	-	-	-		-	-			0.5			16	18.4		16.8	31	.7	2.5	.7	12.2		
SiH_4, mole %	-	-	-		-	-			-			20	9.4		67.6	5.1	.1		99.1	5.1		
HCl, mole %		1.1	-		-	-																

Figure A1.2-1 Process Flow Sheet for Silane Process -CASE B
(Provided by Union Carbide)

CASE B

TABLE A1.2-1 CHEMICAL ENGINEERING ANALYSES: PRELIMINARY PROCESS DESIGN ACTIVITIES FOR SILANE PROCESS-CASE B

Prel. Process Design Activity	Status
1. Specify Base Case Conditions	●
1. Plant Size	●
2. Product Specifics	●
3. Additional Conditions	●
2. Define Reaction Chemistry	●
1. Reactants, Products	●
2. Equilibrium	●
3. Process Flow Diagram	●
1. Flow Sequence, Unit Operations	●
2. Process Conditions (T, P, etc.)	●
3. Environmental	●
4. Company Interaction (Technology Exchange)	●
4. Material Balance Calculations	●
1. Raw Materials	●
2. Products	●
3. By-Products	●
5. Energy Balance Calculations	●
1. Heating	●
2. Cooling	●
3. Additional	●
6. Property Data	●
1. Physical	●
2. Thermodynamic	●
3. Additional	●

Prel. Process Design Activity	Status
7. Equipment Design Calculations	●
1. Storage Vessels	●
2. Unit Operations Equipment	●
3. Process Data (P, T, rate, etc.)	●
4. Additional	●
8. List of Major Process Equipment	●
1. Size	●
2. Type	●
3. Materials of Construction	●
8a. Major Technical Factors	●
(Potential Problem Areas)	●
1. Materials Compatibility	●
2. Process Conditions Limitations	●
3. Additional	●
9. Production Labor Requirements	●
1. Process Technology	●
2. Production Volume	●
10. Forward for Economic Analysis	●

0 Plan
◐ In Progress
● Complete

CASE B

TABLE A1.2-2

BASE CASE CONDITIONS FOR SILANE PROCESS-CASE B

1. Plant Size
   - Allow for 10% losses of silane in production of silicon
   - 1270 metric tons/year of silane
   - Solar cell grade silicon

2. Hydrogenation Reaction
   - Metallurgical grade silicon, hydrogen, to produce trichlorosilane (TCS) make-up hydrogen chloride used and recycle silicon tetrachloride (TET)
   - Copper catalyzed
   - Fluidized bed
   - 550°C, 50 PSIG
   - 15.8% conversion of $SiCl_4$ (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)
   - Conversion from pure TCS feed is about 10% to DCS (example)
4. DCS Redistribution Reaction
   - DCS produces 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-1.1 (Union Carbide equilibrium)
   - Conversion from pure DCS feed is about 14% to Silane (example)
5. Recycles
   - Unreacted chlorosilanes separated by distillation and recycled

6. Silane Purification
   - Chlorosilanes removed by absorption in -40°C $SiCl_4$ (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)

CASE B

TABLE A1.2-3

REACTION CHEMISTRY FOR SILANE PROCESS - CASE B

1. Hydrogenation Reaction

$$3\ SiCl_4 + Si + 2H_2 \rightleftarrows 4SiHCl_3$$

2. Trichlorosilane Redistribution Reaction

$$2\ SiHCl_3 \rightleftarrows SiH_2Cl_2 + SiCl_4$$

3. Dichlorosilane Redistribution Reaction

$$3\ SiH_2Cl_2 \xrightarrow{\text{Distillation}} 2SiHCl_3 + SiH_4$$

Note

1. Reaction 1 Product contains H_2, $SiCl_4$, $SiHCl_3$, SiH_2Cl_2 (trace), other trace chlorides
2. Reaction 2 Product contains $SiHCl_3$, $SiCl_4$, SiH_2Cl_2, SiH_3Cl
3. Reaction 3 Product contains SiH_2Cl_2, $SiHCl_3$, $SiCl_4$, SiH_3Cl, SiH_4

CASE B

TABLE A1.2-4

RAW MATERIAL REQUIREMENTS FOR SILANE PROCESS-CASE B

Raw Material	Requirement lb/lb of Silane
1. Anhydrous HCl	1.239
2. Hydrogen	.362
3. Caustic (50%)	2.448
4. M.G. Silicon	1.11

CASE B

TABLE A1.2-5

UTILITY REQUIREMENTS FOR SILANE PROCESS - CASE B

	Utility/Function	Requirements/lb of Silane Product	
1.	Electricity		.212 KW-HR
	1. All pump and Compressor Motors (16)	.212)	
2.	Steam 250 Psia		186.72 lbs
	1. #1 Distillation Column Preheater	(6.96)	
	2. #1 Distillation Column Reboiler	(81.18)	
	3. #2 Distillation Column Reboiler	(91.77)	
	4. #2 Redistribution Reacotr Preheater	(3.0)	
	5. #3 Distillation Column Reboiler	(3.29)	
	6. #4 Distillation Column Reboiler	(0.41)	
	7. Waste Treatment	(0.11)	
3.	Cooling Water (10-120°F)		168.12 gallons
	1. #1 Distillation Column Condenser	(146.12)	
	2. #2 Distillation Column Condenser	(22.09)	
4.	Process Water (90°F)		8.22 gallons
	1. Waste Treatment	(8.22)	
5.	Refrigerant (-20°F)		2303.2 BTU
	1. #3 Distillation Column Condenser	(2058.0)	
	2. #4 Distillation Column Condenser	(245.2)	
6.	Refrigerant (-30°F)		30788.0 BTU
	1. TCS Reactor Recycle Gas Condenser	(30788.0)	
7.	Refrigerant (-40°F)		25.26 BTU
	1. Silane Product Storage	(25.26)	
8.	Refrigerant (-50°F)		517.2 BTU
	1. Product Silane Condenser	(137.9)	
	2. Absorbent Cooler	(379.3)	
9.	High Temperature Heat Exchange Fluid		3.324×10^4 BTU
	1. TCS Reactor Recycle Gas Heater	(6.591×10^3)	
	2. HCl Vaporizer	(4.46×10^2)	
	3. Tet Vaporizer	(2.464×10^4)	
	4. Heat Nitrogen to Regenerate Char. Adsorbers	(70.95)	
	5. TCS Reactor	(1.491×10^3)	

CASE B

TABLE A1.2-5 (Continued)

Utility/Function		Requirements/lb of Silane Product
10. Nitrogen		5.54 SCF
1. Regenerate Charcoal Adsorbers	(5.54)	

CASE B

TABLE A1.2-6

LIST OF MAJOR PROCESS EQUIPMENT FOR SILANE PROCESS - CASE B

		Type	Function	Duty	Size	Materials of Construction
1.	(T1)	M.G. Silicon Storage Hopper	Raw Material Storage	2 weeks storage	1.363×10^4 gallons	CS
2.	(T2)	Hydrogen Storage Tank	Raw Material Storage	8 hours backup for pipeline failure	9.161×10^4 gallons 250 PSIA (spherical)	CS
3.	(T3)	Liquid HCl Storage Tank	Raw Material Storage	2 weeks storage	1.612×10^4 gallons 250 PSIA, -50°F (spherical)	Nickel Steel
4.	(T4)	Recycle TET Storage	For TCS REactor Feed	1 day storage	9.923×10^4 gallons 65 PSIA	CS
5.	(T5)	TCS Reactor Off-Gas Flash Tank	Phase Separation		1 ft. diameter by 4 ft. long, 65 PSIA, 0°F 65 PSIA	CS
6.	(T6)	TCS/TET Storage	Feed Distillation Column #1	1 day hold-up	1.966×10^5 65 PSIA	CS
7.	(T7)	#1 Distillation Column Condensate Accumulator	Reflux feed; column Control	20 minutes hold-up	4.88×10^3 gallons 65 PSIA	CS
8.	(T8)	#2 Distillation Column Condensate Accumulator	Reflux feed; column Control	20 minutes hold-up	746 gallons 65 PSIA	SS
9.	(T9)	#3 Distillation Column Condensate Accumulator	Reflux feed; phase Separation; column control	20 minutes hold-up	194 gallons 5°F. 60 PSIA	SS

CASE B

TABLE A1.2-6 (Continued)

10.	(T10)	#4 Distillation Column Condensate Tank	Reflux feed; column control	20 minutes hold-up	18 gallons 50 PSIA, -7°F	SS
11.	(T11)	Waste Tank	Collect waste for Treatment and disposal	2 week storage	1.378 x 10^4 gallons 65 PSIA	CS
12.	(T12)	Silane Storage	Final Product Storage	2 days storage 8.97 x 10^3 BTU/Hr	4.349 x 10^3 gallons -40°F, 250 PSIA	SS
13.	(T13)	Caustic Storage	Raw Material Storage	2 weeks storage	2.304 x 10^4 gallons	SS
14.	(H1)	TCS Reactor Recycle Gas Heater	Heat Recycle gas and Hydrogen to 550°C	2.342 x 10^6 BTU/hr	752 ft^2 65 PSIA	CS
15.	(H2)	HCl Vaporizer	Heat Reactant to 550°C	1.587 x 10^5 BTU/hr	34 Ft^2 65 PSIA	CS
16.	(H3)	TET Vaporizer	Heat Reactant to 550°C	8.755 x 10^6 BTU/hr	2381 ft^2 65 PSIA	CS
17.	(H4)	TCS Teactor Recycle Condenser	Phase separation; Recycle hydrogen	1.094 x 10^7 BTU/hr	1882 ft^2 65 PSIA	CS/SS
18.	(H5)	#1 Distillation Column Preheater	Preheat distillation feed to bubble point	2.044 x 10^6 BTU/hr	164 ft^2 250 PSIA	CS
19.	(H6)	#1 Distilllation Column Condenser	Provide Reflux to Column	1.296 x 10^7 BTU/hr	3189 ft^2 65 PSIA	CS
20.	(H7)	#1 Distillation Column Reboiler	Provide vapor to Column	2.382 x 10^7 BTU/hr	2818 ft^2 250 PSIA	CS

CASE B

TABLE A1.2-6 (Continued)

21.	(H8)	#2 Distillation Column Condenser	Provide Reflux to column	1.96×10^6 BTU/hr	956 ft^2 65 PSIA	CS/SS
22.	(H9)	#2 Distillation Column Reboiler	Provide Vapor to column	2.693×10^7 BTU/hr	2514 ft^2 250 PSIA	CS
23.	(H10)	#2 Redistribution Reactor Feed Vaporizer	Vaporize Reactants for Reactor	8.81×10^5 BTU/hr	78 ft^2 250 PSIA	CS/SS
24.	(H11)	#3 Distillation Column Condenser	Provide Column Reflux (Partial Condenser)	7.312×10^5 BTU/hr	593 ft^2 60 PSIA	CS/SS
25.	(H12)	#3 Distillation Column Reboiler	Provide Vapor to Column	9.64×10^5 BTU/hr	84 ft^2 250 PSIA	CS/SS
26.	(H13)	Silane Condenser	Condense Final Product for storage	4.9×10^4 BTU/hr	53 ft^2 250 PSIA	CS/SS
27.	(H14)	#4 Distillation Column Condenser	Provide Reflux	8.71×10^4 BTU/hr	84 ft^2 50 PSIA	CS/SS
28.	(H15)	#4 Distillation Column Reboiler	Provide Vapor to Column	1.2×10^5 BTU/hr	13 ft^2 250 PSIA	CS/SS
29.	(H16)	Absorber Precooler	Cool TET for absorption column	1.35×10^5 BTU/hr	35 ft^2 60 PSIA	CS/SS
30.	(H17)	Nitrogen Heater	Heat Nitrogen to regenerate Charcoal Adsorbers	2.52×10^4 BTU/hr	14.1 ft^2	CS
31.	(P1)	TCS Reactor Off Gas Recycle Compressor	Circulate Recycle Gas to Reactor	1.36×10^3 SCFM	26.5 Horsepower 75 PSIA Discharge	CS*

CASE B

TABLE A1.2-6 (Continued)

32.	(P2)	#1 Distillation Column Feed Pump	Feed Column	136.5 gpm	106 PSI; 14.5 BHP	CS*
33.	(P3)	#1 Distillation Column Overheads Pump	Provide Reflux and remove overhead product	244 gpm	92.3 PSI; 22.5 BHP	CS*
34.	(P4)	#1 Distillation Column Bottoms Pump	Remove Bottoms Product to TET storage tank	69 gpm	106 PSI, 7.3 BHP	CS*
35.	(P5)	Process Water Feed Pump	Feed Process Water to Waste Treatment	48.6 gpm	82.5 PSI; 4 BHP	CS*
36.	(P6)	Caustic Feed	Feed Raw Material	1 gpm	118 PSI; 1/4 BHP	SS
37.	(P7)	#2 Distillation Column Overheads Pump	Provide Reflux and Remove Overhead Product	37.3 gpm	92.3 PSI; 3.4 BPH	SS
38.	(P8)	#2 Distillation Column Bottoms Pump	Remove Bottoms Product to TCS/TET storage tank	66.7 gpm	106.3 PSI; 7.1 BPH	SS
39.	(P9)	#3 Distillation Column Overhead Pump	Provide Reflux; Remove Overhead Product	9.7 gpm	87.3 PSI; 1 BHP	SS
40.	(P10)	#3 Distillation Column Bottoms Pump	Remove Bottoms Product to TCS/TET Tank	5.2 gpm	106.3 PSI; 1/2 BHP	SS

* Includes incremental higher cost for special purity requirements.

<u>CASE B</u>

TABLE A1.2-6 (Continued)

41.	(P11)	#4 Distillation Column Overhead Pump	Provide Reflux, Remove Overhead Product	1 gpm	77.3 PSI; 1/4 BHP	SS
42.	(P12)	#4 Distillation Column Bottoms Pump	Remove Bottoms Product to Absorber Feed Tank	1 gpm	91.3 PSI; 1/4 BHP	SS
43.	(P13)	Silane Product Compressor	Liquefy Silane for Storage	66 SCFM	250 PSIA Discharge 6.5 HP	SS
44.	(P14)	Waste Feed Pump	Distillation Wastes to Waste Treatment	1 gpm	76.3 PSI; 1/4 BHP	CS
45.	(P15)	TCS Reactor Feed Pump	Feed TET to Reactor	69 gpm	92.3 PSI; 6.4 BHP	CS*
46.	P16)	Waste Collection Pump	Distillation Wastes to Waste Tank	1 gpm	87.3 PSI; 1/4 BHP	CS
47.	(C1)	#1 Distillation Column	Separate TET from TCS	94,220 lb/hr of feed	7.56 ft. diameter 100 ft. tall, 50 trays	CS
48.	(C2)	#2 Distillation Column	Separate TCS from DCS	48,321 lb/hr of feed	10.6 ft. Diameter 136 ft. tall, 68 trays	CS
49.	(C3)	#3 Distillation Column	Separate Silane from other Chlorosilanes	7344 lb/hr of feed	2.01 ft. Diameter 29 ft. tall, 29 trays	SS
50.	(C4)	#4 Distillation Column	Strip TET for use in absorber	1007.7 lb/hr of feed	1.04 ft. Diameter 28.5 ft. tall, 38 trays	SS
51.	(C5)	Silane Absorber	Absorb Chlorosilane from Silane	819.3 lb/hr of vapor feed	0.823 ft. Diameter 12 ft. tall, 16 trays	SS

* Includes incremental higher cost for special purity requirements.

CASE B

TABLE A1.2-6 (Continued)

52.	(C[illegible])	Charcoal Adsorber	Activated Carbon Adsorbtion of Silane to remove Trace Chlorosilane	366 lb/hr of vapor feed	1 ft. Diameter 7 ft. tall (2), 623 lbs of carbon	SS
53.	(R1)	TCS Fluidized Bed Reactor	Produces TCS from TET,M.G. Silicon, and H_2		6.26 ft. in Diameter 26.5 ft. tall, 481 tubes 1", 16' long	SS
54.	(R2)	#1 Redistribution Reactor (2)	Redistribute TCS to DCS		2' Diameter by 15 ft. tall 1042 lbs catalyst	SS
55.	(R3)	#2 Redistribution Teactor (2)	Redistribute [illegible] to Silane		2.34' Diameter by 35 ft. tall 1667.2 lbs catalyst	SS
56.	(A1)	Fines Separator	Remove Silicon Fines carried over with TCS Reactor Off-gas		Standard design 30" Diameter	SS
57.	(A2)	Waste Treatment	Discharge innocuous effluent		1 column for adsorption + 1 heat exchanger to vaporize feed	SS
58.	(A3)	Hydrogen Flare	Dispose of Hydrogen from Waste Treatment		30 ft. stack 6" Diameter	CS

CASE B

TABLE A1.2-7

PRODUCTION LABOR REQUIREMENTS FOR SILANE PROCESS - CASE B

	Unit Operation	Type	Skilled Labor, Man Hours Per Day	Skilled Labor, Man Hours Per lb. Silane
1.	TCS Production	B	65	.0085
2.	Hydrogen Recycle	C	18	.0023
3.	Raw Material Vaporization	C	50	.0065
4.	TCS Condensation	C	50	.0065
5.	TCS/TET Separation	C	62	.0081
6.	#1 Redistribution Reactor	C	49	.0064
7.	DCS/TCS Separation	C	52	.0068
8.	#2 Redistribution Reactor	C	32	.0042
9.	Silane Distillation	C	32	.0042
10.	Silane Absorption	C	28	.0036
11.	Silane Purification (adsorption)	A	36	.0047
12.	Silane compression	B	23	.003
13.	Silane Condensation	B	23	.003
14.	Materials Handling	A	48*	.0063*
15.	Waste Treatment	B	60	.0078
16.	Silicon Fines Separation	A	15	.002
	TOTAL		595	.0776

NOTES:

1. A Batch Process of Miltiple Small Units
   B Average Process
   C Automated Process

2. Man hours/day unit from Figure 4-6, Peters and Timmerhaus (7).

*semi-skilled

A1.3 Silane Process - Case C

Initial results for the Silane Process (Cases A and B) were marginal and indicated process revisions were warranted.

Based on these initial findings, Union Carbide engineering, research development personnel revised their flowsheet for a more optimum arrangement of major process equipment, raw material requirements and operating conditions. A joint meeting with Union Carbide and Lamar was conducted in late January (1978) for initial review of the revised flowsheet and potential lower plant capital investment and lower product cost for silane production.

In the revised silane process, the silicon tetrachloride is hydrogenated in a fluidized bed of silicon which is catalyzed by copper. The hydrogenation reaction is conducted at a higher pressure than originally proposed to increase the yield of desireable trichlorosilane. The gas leaving the fluidized bed reactor is cooled and condensed to recover the liquid chlorosilanes. The hydrogen is recycled.

The condensed liquid chlorosilanes are separated by distillation. The inerts (dissolved gases) are removed in the initial distillation column. The remaining distillation columns separate the liquid chlorosilanes into primarily silicon tetrachloride, trichlorosilane, dichlorosilane and silane. The silicon tetrachloride is recycled back to the hydrogenation reactor. The trichlorosilane and dichlorosilane are sent to the redistribution reactors for rearrangement of chlorine/hydrogen bonds to silicon. The final redistribution reactor product is sent to the silane distillation column. The silane is removed from this distillation and sent to silicon production.

Chemical engineering analysis results for the Silane Process - Case C (Revised Process) are given in Section 3.3- UCC Silane Process for Silicon (Union Carbide Corporation).

A2. ADDITIONAL ECONOMIC ANALYSIS

A2.1 Silane Process - Case A

The economic analysis activity for the Silane Process -Case A (Regular Process Storage) involves a cost analysis to produce silane for silicon. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silane by the Silane Process - Case A are presented in Table A2.1-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of $5.55 (1975 dollars) and $7.77 (1980 dollars) per lb of silane. This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses. These results, when expressed in terms of silicon contained in the silane, correspond to $13.94 (1975 dollars) and $19.53 (1980 dollars) per kg of silicon.

This cost results for the Silane Process - Case A indicate that this new technology for producing silane for silicon is marginal. Revisions are warranted for meeting the cost goal of $14 per kg of silicon material (1980 dollars) for solar cells.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

Preliminary Economic Analysis Activities	Table A2.1-2
Process Design Inputs	Table A2.1-3
Base Case Conditions	Table A2.1-4
Raw Material Cost	Table A2.1-5
Utility Cost	Table A2.1-6
Major Process Equipment Cost	Table A2.1-7
Production Labor Cost	Table A2.1-8
Plant Investment	Table A2.1-9
Total Product Cost	Table A2.1-10

TABLE A2.1-1

ESTIMATION OF PRODUCT COST FOR SILANE PROCESS - CASE A

	Cost $/lb of Silane (1975 dollars)	Cost $/lb of Silane (1980 dollars)
1. Direct Manufacturing Cost (Direct Costs)......	3.34	4.68
Raw Materials		
Direct Operating Labor		
Utilities		
Supervision and Clerical		
Maintenance and Repairs		
Operating Supplies		
Laboratory Charge		
2. Indirect Manufactuing Cost (Fixed Cost).......	0.89	1.25
Depreciation		
Local Taxes		
Insurance		
3. Plant Overhead................................	0.60	.84
4. General Expenses..............................	0.72	1.01
Administration		
Distribution and Sales		
Research and Development		
5. Product Cost Without Profit..................	5.55	7.77

CASE A

Table A2.1-2

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITIES FOR SILANE PROCESS
CASE A

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	
1. Base Year for Costs	●
2. Appropriate Indices for Costs	●
3. Additional	●
3. Raw Material Costs	●
1. Base Cost/lb. of Material	●
2. Material Cost/lb of Silane	●
3. Total Cost/lb of Silane	●
4. Utility Costs	●
1. Base Cost for Each Utility	●
2. Utility Cost/lb of Silane	●
3. Total Cost/lb of Silane	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost/lb Silane Per Area	●
3. Total Cost/lb Silane	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○	Plan
◐	In Progress
●	Complete

TABLE A2.1-3

PROCESS DESIGN INPUTS FOR SILANE PROCESS - CASE A

1. Raw Material Requirements
   -M.G. Silicon, anhydrous HCl, caustic, hydrogen.
   -see table for "Raw Material Cost"
2. Utility
   -electrical, steam, cooling water, etc.
   -see table for "Utility Cost"
3. Equipment List
   -76 pieces of major process equipment
   -process vessels, heat exchangers, reactor, etc.
   -see table for "Major Process Equipment Cost"
4. Labor Requirements
   -production labor for purification, vaporization, product handling, etc.
   -see table for "Production Labor Cost"

<u>CASE A</u>

TABLE A2.1-4

BASE CASE CONDITIONS FOR
SILANE PROCESS-CASE A

1. Capital Equipment

   -January 1975 Cost Index for Capital Equipment Cost
   -January 1974 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

3. Raw Material Cost

   -Chemical Marketing Reporter
   -January 1975 Value
   -Other Sources

4. Labor Cost

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

5. Update to 1980

   historically cite 1975 dollars (LSA project)
   JPL decision to change to 1980 dollars (JPL, 6/22/79)
   -reports to reflect <u>both</u> 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

CASE A

TABLE A2.1-5

RAW MATERIAL COST FOR SILANE PROCESS - CASE A

Raw Material	Requirement lb/lb of Silane	$/lb of Material	Cost $/lb of Silane
1. HCl	1.239	.10	.12
2. Hydrogen	.362	.96	.35
3. Caustic (50%)	2.448	.0382	.09
4. M.G. Silicon	1.11	.454	.50
			1.06 (1975 dollars)
			x 1.4 inflation
			1.48 (1980 dollars)

CASE A

TABLE A2.3-6

UTILITY COST FOR SILANE PROCESS -CASE A

	Utility	Requirement/lb of Silane	Cost of Utility	Cost $/lb of Silane
1.	Electricty	.253 Kw-Hr	$.03/KW hr	.0076
2.	Steam	190.34 lbs	1.25/M lb	.2379
3	Cooling Water	168.12 gallons	.08/M gal	.0134
4.	Process water	8.22 gallons	.35/M gal	.0029
5.	Refrigerant (23°F)	27.1 BTU	4.[illegible]/MM BTU	.0001
6.	Refrigerant (5°F)	79.1 BTU	6.40/MM BTU	.0005
7.	Refrigerant (-7°F)	26.4 BTU	7.50/MM BTU	.0002
8.	Refrigerant (-20°F)	2.3 M BTU	8.70/MM BTU	.0200
9.	Refrigerant (-30°F)	30.8 M BTU	9.60/MM BTU	.2957
10.	Refrigerant (-40°F)	369 BTU	10.50/MM BTU	.0039
11.	Refrigerant (-50°F)	3.5 M BTU	11.40/MM BTU	.0400
12.	High Temperature Heat Exchange Fluid	3.324×10^4 BTU	3.0/MM BTU	.099
13.	Nitrogen	5.54 SCF	.50/M SCF	.0028

.724 (1975 dollars)
x 1.4 inflation
1.01 (1980 dollars)

CASE A

TABLE A2.1-7

PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR SILANE PROCESS-CASE A

	Equipment		Purchased Cost,$1000
1.	(T1)	M.G. Silicon Storage Hopper	12.05
2.	(T2)	Hydrogen Storage Tank	179.2
3.	(T3)	Liquid HCl Storage Tank	95.27
4.	(T4)	Recycle TET Storage	214,4
5.	(T5)	TCS Reactor Off-Gas Flash Tank	0.71
6.	(T6)	TCS/TET Storage	214.4
7.	(T7)	#1 Distillation Column Condensate Accumlator	8.51
8.	(T8)	#1 Redistribution Reactor Feed Tank	241.99
9.	(T9)	#1 Redistribution Reactor Product Tank	248.0
10.	(T10)	#2 Distillation Column Condensate Accumulator	7.37
11.	(T11)	#2 Redistribution Reactor Feed Tank	76.03
12.	(T12)	#2 Redistribution Reactor Product Tank	221.17
13.	(T13)	#3 Distillation Column Condensate Accumulator	2.76
14.	(T14)	#3 Distillation Column Condensate Tank	147.44
15.	(T15)	#4 Distillation Column Feed Tank	53.45
16.	(T16)	#4 Distillation Column Condensate Accumulator	2.76
17.	(T17)	#4 Distillation Column Condensate Tank	34.1
18.	(T18)	Waste Tank	17.01
19.	(T19)	Absorber Feed Tank	16.59
20.	(T20)	Silane Storage	255.9
21.	(T21)	Caustic Storage	92.15
22.	(H1)	TCS Reactor Recycle Gas Heater	8.12
23.	(H2)	HCl Vaporizer	1.15
24.	(H3)	TET Vaporizer	18.48
25.	(H4)	TCS Reactor Recycle Condenser	38.98

CASE A

TABLE A2.1-7 (continued)

26.	(H5)	#1 Distillation Column Preheater	3.24
27.	(H6)	#1 Distillation Column Condenser	22.4
28.	(H7)	#1 Distillation Column Reboiler	23.7
29.	(H8)	#2 Distillation Column Condenser	21.08
30.	(H9)	#2 Distillation Column Reboiler	21.16
31.	(H10)	#2 Redistribution Reactor Feed Vaporizer	3.67
32.	(H11)	#2 Redistribution Reactor Product condenser	8.62
33.	(H12)	#3 Distillation Column Preheater	2.86
34.	(H13)	#3 Distillation Column Condenser	14.95
35.	(H14)	#3 Distillation Column Reboiler	3.88
36.	(H15)	Silane Condenser	2.29
37.	(H16)	#4 Distillation Column Condenser	3.48
38.	(H17)	#4 Distillation Column Reboiler	1.33
39.	(H18)	Absorber Pre-cooler	1.79
40.	(H19)	Nitrogen Heater	.92
41.	(P1)	TCS Reactor Off-gas Recycle Compressor	35.1
42.	(P2)	#1 Distillation Column Feed Pump	5.03
43.	(P3)	#1 Distillation Column Overheads Pump	6.04
44.	(P4)	#1 Distillation Colum Bottoms Pump	3.59
45.	(P5)	Process Water Feed Pump	2.87
46.	(P6)	Caustic Feed Pump	1.25
47.	(P7)	#1 Redistribution Reactor Feed Pump	4.02
48.	(P8)	#2 Distillation Column Feed Pump	3.59
49.	(P9)	#2 Distillation Column Overheads Pump	2.57
50.	(P10)	#2 Distillation Column Bottoms Pump	3.59
51.	(P11)	#2 Redistribution Reactor Feed Pump	2.09
52.	(P12)	#3 Distillation Column Feed Pump	1.77

CASE A

TABLE A2.1-7 (continued)

53.	(P13)	#3 Distillation Column Overheads Pump	1.77
54.	(P14)	#3 Distillation Column Bottoms Pump	1.47
55.	(P15)	#4 Distillation Column Feed Pump	1.23
56.	(P16)	#4 Distillation Column Overheads Pump	1.23
57.	(P17)	#4 Distillation Column Bottoms Pump	1.23
58.	(P18)	#4 Distillation Condensate Recycle Pump	1.23
59.	(P19)	Silane Product Compressor	17.55
60.	(P20)	Waste Feed Pump	.62
61.	(P21)	TCS Reactor Feed Pump	3.31
62.	(P22)	#3 Distillation Condensate Recycle Pump	1.47
63.	(P23)	Waste Collection Pump	.62
64.	(P24)	Absorber Feed Pump	1.23
65.	(C1)	#1 Distillation Column	100.66
66.	(C2)	#2 Distillation Column	214.08
67.	(C3)	#3 Distillation Column	40.19
68.	(C4)	#4 Distillation Column	21.14
69.	(C5)	Silane Absorber	15.06
70.	(C6)	Charcoal Adsorber	18.0
71.	(R1)	TCS Fluidized Bed Reactor	155.06
72.	(R2)	#1 Redistribution Reactor	13.26
73.	(R3)	#2 Redistribution Reactor	33.14
74.	(A1)	Fines Separator	2.0
75.	(A2)	Waste Treatment	18.72
76.	(A3)	Hydrogen Flare	0.10

TOTAL PURCHASED EQUIPMENT COST $3079.31 (1975 dollars)
x 1.4 inflation
4,311.03 (1980 dollars)

CASE A

TABLE A2.1-8

PRODUCTION LABOR COST FOR SILANE PROCESS - CASE A

	Unit Operation	Skilled Labor Man-Hrs/lb Silane	Cost $/lb of Silane
1.	TCS Production	.0085	.05865
2.	Hydrogen Recycle	.0023	.01587
3.	Raw Material Vaporization	.0065	.04485
4.	TCS Condensation	.0065	.04485
5.	TCS/TET Separation	.0081	.05589
6.	#1 Redistribution Reactor	.0064	.04416
7.	DCS/TCS Separation	.0068	.04692
8.	#2 Redistribution Reactor	.0042	.02898
9.	Silane Distillation	.0042	.02898
10.	Silane Absorption	.0036	.02484
11.	Silane Purification(Adsorption)	.0047	.03243
12.	Silane Compression	.003	.0207
13.	Silane Condensation	.003	.0207
14.	Materials Handling	.0063*	.03087
15.	Waste Treatment	.0078	.05382
16.	Silicon Fines Separation	.002	.0138
			$.5663 (1975 dollars)
			x 1.4 inflation
			.7928 (1980 dollars)

NOTES

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

* Semiskilled Labor

TABLE A2.1-9

ESTIMATION OF PLANT INVESTMENT FOR SILANE PROCESS - CASE A

	Investment $1000
1. DIRECT PLANT INVESTMENT COSTS	
1. Major Process Equipment Cost	$3079.31
2. Installation of Major Process Equipment	1324.10
3. Process Piping, Installed	2278.69
4. Instrumentation, Installed	585.07
5. Electrical, Installed	307.93
6. Process Buildings, Installed	307.93
1a. SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	7883.03
2. OTHER DIRECT PLANT INVESTMENT COSTS	
1. Utilities, Installed	1478.07
2. General Services, Site Development, Fire Protection, etc.	369.52
3. General Buildings, Offices, Shops, etc.	431.10
4. Receiving, Shipping Facilities	646.66
2a. SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	2925.35
3. TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	10808.38
4. INDIRECT PLANT INVESTMENT COSTS	
1. Engineering, Overhead, etc.	1693.62
2. Normal Cont. for Floods, Strikes, etc.	2186.31
4a. TOTAL INDIRECT PLANT INVESTMENT COST	3879.93
5. TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	14688.31
6. OVERALL CONTINGENCY	4406.49
7. FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	19094.80 (1975 dollars)
	x 1.4 inflation
	26732.72 (1980 dollars)

CASE A

TABLE A2.1-10

ESTIMATION OF TOTAL PRODUCT COST FOR SILANE PROCESS- CASE A

		$/lb of Silane
1.	Direct Manfacturing Cost (Direct Charges)	
	1. Raw Materials- from prel. design	1.06
	2. Direct Operating Labor- from prel. design	.5663
	3. Utilities-from prel. design	.724
	4. Supervision and Clerical,	.085
	5. Maintenance and Repairs,	.682
	6. Operating Supplies,	.136
	7. Laboratory Charge,	.085
	8. Patents and Royalties, costs	----
2.	Indirect Manufacturing Cost (Fixed Charges)	
	1. Depreciation	.682
	2. Local Taxes	.136
	3. Insurance	.068
	4. Interest	----
3.	Plant Overhead	.595
4.	By-Product Credit- from prel. design	--
4a.	Total Manufacturing Cost, 1 + 2 + 3 + 4	4.819
5.	General Expenses	
	1. Administration,	.289
	2. Distribution and Sales, cost	.289
	3. Research and Development, cost	.145
6.	Total Cost of Product, 4a + 5	5.55 (1975 dollars) x 1.4 inflation 7.77 (1980 dollars)

A2.2 Silane Process - Case B

The economic analysis activity for the Silane Process -Case B (Minimum Process Storage) involves a cost analysis to produce silane for silicon. Primary results issuing from the economic analysis include plant capital investment and product cost which are useful in identification of those processes showing promise for meeting project cost goals.

The cost analysis results for producing silane by the Silane Process - Case B are presented in Table A2.2-1 including costs for raw materials, labor, utilities and other items composing the product cost (total cost of producing silicon). The tabulation summarizes all of these items to give a total product cost without profit of \$4.58 (1975 dollars) and \$6.41 (1980 dollars) per lb of silane. These results, when expressed in terms of silicon contained in the silane, correspond to \$11.53 (1975 dollars) and \$16.12 (1980 dollars) per kg of silicon.

These cost results for the Silane Process-Case B indicate that this new technology for producing silane for silicon is marginal. Revisions are warranted for meeting the cost goal of \$14 per kg of silicon material (1980 dollars) for solar cells.

The detailed results for the economic analysis are presented in a tabular format to make it easier to locate cost items of specific interest. The guide for the tabular format is given below:

Preliminary Economic Analysis Activities..	Table A2.2-2
Process Design Inputs....................	Table A2.2-3
Base Case Conditions.....................	Table A2.2-4
Raw Material Cost........................	Table A2.2-5
Utility Cost.............................	Table A2.2-6
Major Process Equipment..................	Table A2.2-7
Production Labor Cost....................	Table A2.2-8
Plant Investment.........................	Table A2.2-9
Total Product Cost.......................	Table A2.2-10

TABLE A2.2-1

ESTIMATION OF PRODUCT COST FOR SILANE PROCESS - CASE B

		Cost $/lb of Silane (1975 dollars)	Cost $/lb of Silane (1980 dollars)
1.	Direct Manufacturing Cost (Direct Costs)......	2.95	4.13
	Raw Materials		
	Direct Operating Labor		
	Utilities		
	Supervision and Clerical		
	Maintenance and Repairs		
	Operating Supplies		
	Laboratory Charge		
2.	Indirect Manufactuing Cost (Fixed Cost).......	0.52	0.73
	Depreciation		
	Local Taxes		
	Insurance		
3.	Plant Overhead.............................	0.51	0.71
4.	General Expenses...........................	0.60	0.84
	Administration		
	Distribution and Sales		
	Research and Development		
5.	Product Cost Without Profit..................	4.58	6.41

CASE B

TABLE A2.2-2

ECONOMIC ANALYSES:
PRELIMINARY ECONOMIC ANALYSIS ACTIVITES FOR SILANE PROCESS - CASE B (UNION CARBIDE)

Prel. Process Economic Activity	Status
1. Process Design Inputs	●
1. Raw Material Requirements	●
2. Utility Requirements	●
3. Equipment List	●
4. Labor Requirements	●
2. Specify Base Case Conditions	●
1. Base Year for Costs	●
2. Appropriate Indices for Costs	●
3. Additional	●
3. Raw Material Costs	●
1. Base Cost/Lb. of Material	●
2. Material Cost/lb of Silane	●
3. Total Cost/lb of Silane	●
4. Utility Costs	●
1. Base Cost for Each Utility	●
2. Utility Cost/lb of Silane	●
3. Total Cost/lb of Silane	●
5. Major Process Equipment Costs	●
1. Individual Equipment Cost	●
2. Cost Index Adjustment	●

Prel. Process Economic Activity	Status
6. Production Labor Costs	●
1. Base Cost Per Man Hour	●
2. Cost/lb Silane Per Area	●
3. Total Cost/lb Silane	●
7. Estimation of Plant Investment	●
1. Battery Limits Direct Costs	●
2. Other Direct Costs	●
3. Indirect Costs	●
4. Contingency	●
5. Total Plant Investment (Fixed Capital)	●
8. 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	●

○ Plan
◐ In Progress
● Complete

CASE B

TABLE A2.2-3

PROCESS DESIGN INPUTS FOR SILANE PROCESS - CASE B

1. Raw Material Requirements
   - -M.G. Silicon, anhydrous HCl, caustic, hydrogen.
   - -see table for "Raw Material Cost"
2. Utility
   - -electrical, steam, cooling water, etc.
   - -see table for "Utility Cost"
3. Equipment List
   - -58 pieces of major process equipment
   - -process vessels, heat exchangers, reactor, etc.
   - -see table for "Major Process Equipment Cost"
4. Labor Requirements
   - -production labor for purification, vaporization, product handling, etc.
   - -see table for "Production Labor Cost"

CASE B

TABLE A2.2-4

BASE CASE CONDITIONS FOR SILANE PROCESS - CASE B

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

3. Raw Material Cost

   -Chemical Marketing Reporter
   -January 1975 Value
   -Other Sources

4. Labor Cost

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

5. Update to 1980

   -historically cited 1975 dollars (LSA project)
   -DOE decision to change to 1980 dollars (JPL, 6/22/79)
   -reports to reflect <u>both</u> 1975 and 1980 dollars (JPL, 6/22/79)
   -inflation factor of 1.4 to be used (JPL, 6/22/79)

CASE B

TABLE A2.2-5

RAW MATERIAL COST FOR SILANE PROCESS-CASE B

Raw Material	Requirement lb/lb of Silane	$/lb of Material	Cost $/lb of Silane
1. HCl	1.239	.10	.12
2. Hydrogen	.362	.96	.35
3. Caustic (50%)	2.448	.0382	.09
4. M.G. Silicon	1.11	.454	.50
			1.06 (1975 dollars)
			x 1.4 inflation
			1.48 (1980 dollars)

CASE B

TABLE A2.2-6

UTILITY COST FOR SILANE PROCESS -CASE B

	Utility	Requirement/lb of Silane	Cost of Utility	Cost $/lb of Silane
1.	Electricty	.212 KW-Hr	$ .03/kw hr	.0064
2.	Steam	186.72 lbs	1.25/M lb	.2334
3.	Cooling Water	168.12 gallons	.08/M gal	.0134
4.	Process Water	8.22 gallons	.35/M gal	.0029
5.	Refrigerant (-20°F)	2.3 M BTU	8.70/MM BTU	.0200
6.	Refrigerant (-30°F)	30.8 M BTU	9.60/MM BTU	.2957
7.	Refrigerant (-40°F)	25.3 BTU	10.50/MM BTU	.0003
8.	Refrigerant (-50°F)	517.2 BTU	11.42/MM BTU	.0059
9.	High Temperature Heat Exchange Fluid	33.24 M BTU	3.0/MM BTU	.0997
10.	Nitrogen	5.54 SCF	.50/M SCF	.0028

.6805 (1975 dollars)
x 1.4 inflation
.9527 (1980 dollars)

CASE B

TABLE A2.2-7

PURCHASED COST OF MAJOR PROCESS EQUIPMENT FOR SILANE PROCESS - CASE B

	Equipment	Purchased Cost, $1000
1.	(T1) M.G. Silicon Storage Hopper	12.05
2.	(T2) Hydrogen Storage Tank	179.2
3.	(T3) Liquid HCl Storage Tank	95.27
4.	(T4) Recycle TET Storage	125.55
5.	(T5) TCS Reactor Off-Gas Flash Tank	0.71
6.	(T6) TCS/TET Storage	214.4
7.	(T7) #1 Distillation Column Condensate Accumulator	8.51
8.	(T8) #2 Distillation Column Condensate Accumulator	7.37
9.	(T9) #3 Distillation Column Condensate Accumulator	2.76
10.	(T10) #4 Distillation Column Condensate Accumulator	2.76
11.	(T11) Waste Tank	17.01
12.	(T12) Silane Storage	82.09
13.	(T13) Caustic Storage	92.15
14.	(H1) TCS Reactor Recycle Gas Heater	8.12
15.	(H2) HCl Vaporizer	1.15
16.	(H3) TET Vaporizer	18.48
17.	(H4) TCS Reactor Recycle Condenser	38.98
18.	(H5) #1 Distillation Column Preheater	3.24
19.	(H6) #1 Distillation Column Condenser	22.4
20.	(H7) #1 Distillation Column Reboiler	23.7
21.	(H8) #2 Distillation Column Condenser	21.08

CASE B

TABLE A2.2-7 (Continued)

22.	(H9)	#2 Distilation Column Reboiler	21.16
23.	(H10)	#2 Redistribulton Reactor Feed Vaporizer	3.67
24.	(H11)	#3 Distillation Column Condenser	14.95
25.	(H12)	#3 Distillation Column Reboiler	3.88
26.	(H13)	Silane Condenser	2.29
27.	(H14)	#4 Distillation Column Condenser	3.48
28.	(H15)	#4 Distillation Column Reboiler	1.33
29.	(H16)	Absorber Pre-cooler	1.79
30.	(H17)	Nitrogen Heater	.92
31.	(P1)	TCS Reactor Off-gas Recycle Compressor	35.1
32.	(P2)	#1 Distillation Column Feed Pump	5.03
33.	(P3)	#1 Distillation Column Overheads Pump	6.04
34.	(P4)	#1 Distillation Column Bottoms Pump	3.59
35.	(P5)	Process Water Feed Pump	2.87
36.	(P6)	Caustic Feed Pump	1.25
37.	(P7)	#2 Distillation Column Overheads Pump	2.57
38.	(P8)	#2 Distillation Column Bottoms Pump	3.59
39.	(P9)	#3 Distillation column Overheads Pump	1.77
40.	(P10)	#3 Distillation Column Bottoms Pump	1.47
41.	(P11)	#4 Distillation Column Overheads Pump	1.23
42.	(P12)	#4 Distillation Column Bottoms Pump	1.23
43.	(P13)	Silane Product Compressor	17.55
44.	(P14)	Waste Feed Pump	.62

CASE B

TABLE A2.2-7 (Continued)

45.	(P15)	TCS Reactor Feed Pump	3.31
46.	(P16)	Waste Collection Pump	.62
47.	(C1)	#1 Distillation Column	100.66
48.	(C2)	#2 Distillation Column	214.08
49.	(C3)	#3 Distillation Column	40.19
50.	(C4)	#4 Distillation Column	21.14
51.	(C5)	Silane Absorber	15.06
52.	(C6)	Charcoal Adsorber	18.0
53.	(R1)	TCS Fluidized Bed Reactor	155.06
54.	(R2)	#1 Redistribuiton Reactor	26.52
55.	(R3)	#2 Redistribution Reactor	66.28
56.	(A1)	Fines Separator	2.0
57.	(A2)	Waste Treatment	18.72
58.	(A3)	Hydrogen Flare	0.10

TOTAL PURCHASED EQUIPMENT COST	1796.17	(1975 dollars)
	x 1.4	inflation
	2515	(1980 dollars)

CASE B

TABLE A2.2-8

PRODUCTION LABOR COST FOR SILANE PROCESS - CASE B

	Unit Operation	Skilled Labor Man-Hrs/lb Silane	Cost $/lb of Silane
1.	TCS Production	.0085	.05865
2.	Hydrogen Recycle	.0023	.01587
3.	Raw Material Vaporization	.0065	.04485
4.	TCS Condensation	.0065	.04485
5.	TCS/TET Separation	.0081	.05589
6.	#1 Redistribution Reactor	.0064	.04416
7.	DCS/TCS Separation	.0068	.04692
8.	#2 Redistribution Reactor	.0042	.02898
9.	Silane Distillation	.0042	.02898
10.	Silane Absorption	.0036	.02484
11.	Silane Purification (Adsorption)	.0047	.03243
12.	Silane Compression	.003	.0207
13.	Silane Condensation	.003	.0207
14.	Materials Handling		.03087
15.	Waste Treatment	.0078	.05382
16.	Silicon Fines Separation	.002	.0138

TOTAL COST .5663 (1975 dollars)
x 1.4 inflation
.7928 (1980 dollars)

NOTES

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

* Semiskilled labor.

CASE B

TABLE A2.2-9

ESTIMATION OF PLANT INVESTMENT FOR SILANE PROCESS - CASE B

		Investment $1000
1.	DIRECT PLANT INVESTMENT COSTS	
	1. Major Process Equipment Cost	$ 1796.17
	2. Installation of Major Process Equipment	772.35
	3. Process Piping, Installed	1329.17
	4. Instrumentation, Installed	341.27
	5. Electrical, Installed	179.62
	6. Process Buildings, Installed	179.62
1a.	SUBTOTAL FOR DIRECT PLANT INVESTMENT COSTS (PRIMARILY BATTERY LIMIT FACILITIES)	4598.2
2.	OTHER DIRECT PLANT INVESTMENT COSTS	
	1. Utilities, Installed	862.16
	2. General Services, Site Development, Fire Protection, etc.	215.54
	3. General Buildings, Offices, Shops, etc.	251.46
	4. Receiving, Shipping Facilities	377.20
2a.	SUBTOTAL FOR OTHER DIRECT PLANT INVESTMENT COSTS (PRIMARILY OFFSITE FACILITIES OUTSIDE BATTERY LIMITS)	1706.36
3.	TOTAL DIRECT PLANT INVESTMENT COST, 1a + 2a	6304.56
4.	INDIRECT PLANT INVESTMENT COSTS	
	1. Engineering, Overhead, etc.	987.89
	2. Normal Cont. for Floods, Strikes, etc.	1275.28
4a.	TOTAL INDIRECT PLANT INVESTMENT COST	2263.17
5.	TOTAL DIRECT AND INDIRECT PLANT INVESTMENT COST, 3 + 4a	8567.73
6.	OVERALL CONTINGENCY	2570.32
7.	FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	11138.05 (1975 dollars) x 1.4 inflation 15593 (1980 dollars)

CASE B

TABLE A2.2-10

ESTIMATION OF TOTAL PRODUCT COST FOR SILANE PROCESS -CASE B

		$/lb of silane
1.	Direct Manfacturing Cost (Direct Charges)	
	1. Raw Materials- from prel. design	1.06
	2. Direct Operating Labor- from prel. design	.5663
	3. Utilities-from prel. design	.6805
	4. Supervision and Clerical,	.0849
	5. Maintenance and Repairs,	.3976
	6. Operating Supplies,	.0795
	7. Laboratory Charge,	.0849
	8. Patents and Royalties, costs	----
2.	Indirect Manufacturing Cost (Fixed Charges)	
	1. Depreciation	.3976
	2. Local Taxes	.0795
	3. Insurance	.0398
	4. Interest	-----
3.	Plant Overhead	.51
4.	By-Product Credit- from prel. design	--
4a.	Total Manufacturing Cost, 1 + 2 + 3 + 4	3.9806
5.	General Expenses	
	1. Administration, cost	.2388
	2. Distribution and Sales, cost	.2388
	3. Research and Development, cost	.1194
6.	Total Cost of Product, 4a + 5	4.58 (1975 dollars) x 1.4 inflation 6.41 (1980 dollars)

A2.3 Silane Process - Case C

Initial cost analysis results for the Silane Process (Cases A and B) were marginal and indicated process revisions were warranted for meeting the project cost goals.

Process revisions were accomplished with favorable cost benefits over the orginal scheme.

The revised process included operation of the silicon tetrachloride reaction at higher pressure for increased trichlorosilane yield should lower recycle requirements. Lower recycle requirements will lower capital equipment and labor costs. The distillation train as now proposed will operate at several hundred pounds pressure compared to original lower pressure. This higher pressure permits use of cooling water in the condensers and does not require expensive low temperature refrigeration as originally proposed. This will provide lower operating (utilities) cost in 3 of the 4 distillation columns. The higher pressure also permits use of smaller diameter columns (vapor loading, density proportional to pressure). The elimination of hydrogen chloride reduces starting material costs. Also, the use of hydrogen from the silane pyrolysis provides additional lower feed material costs.

The revised silane process provided the following cost benefits:

lower capital costs
-lower raw material costs
-lower operating labor costs

Economic analysis results for the Silane Process - Case C (Revised Process) are given in Section 4.3-UCC Silane Process for Silicon (Union Carbide Corporation).