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PROCESS FEASIBILITY STUDY IN SUPPORT OF SILICON
MATERIAL TASK I

Quarterly Technical Progress Report (XX), June 1—August 31, 1980

By
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Issue Date: September 1980

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Carl L. Yaws

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ABSTRACT

Analyses of process system properties were continued for chemical materials important in the production of silicon including compilation and collection activities of the property data for use in the final report. Progress and status are reported for critical constants, vapor pressure, heat of vaporization, heat capacity, density, surface tension, viscosity, thermal conductivity, heat of formation and Gibb's free energy of formation. Compilation and collection activities are about 30% complete covering preparation of the manuscript, figures (graphs) and tables for the final report.

Major efforts in chemical engineering analysis centered on the DCS process - Case A which involves production of dichlorosilane (DCS) as a silicon source material for polysilicon production in the Hemlock Semiconductor Corporation program. The preliminary process design of a plant to produce DCS was completed including process flowsheet (100%), base case conditions (100%), reaction chemistry (100%), raw materials (100%), utilities (100%), major process equipment (100%) and production labor (100%). The process design package was forwarded for economic analysis.

Economic analysis of the DCS process - Case A was completed during this reporting period. The results for dichlorosilane (DCS) indicated a total product cost without profit of 1.29 \$/kg (1980 dollars). This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses. The sales price of DCS at 15% DCF rate of return on investment is 1.47\$/kg (1980 dollars). Additional results are reported for sales price of dichlorosilane at various profitability levels as measured by ROI (return on original investment) and DCF (discounted cash flow rate of return).

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MILESTONE CHART	

I. PROCESS SYSTEM PROPERTIES ANALYSES (TASK 1)

Analyses of process system properties were continued for chemical materials important in the production of silicon including major physical, thermodynamic and transport property data. Primary activities focused on compilation and collection of the property data for use in the final report.

Progress and status in the compilation and collection activities are summarized below:

	<u>Prior</u>	<u>Current</u>
1. Critical Constants	0%	30%
2. Vapor Pressure	0%	30%
3. Heat of Vaporization	0%	30%
4. Heat Capacity	0%	30%
5. Density	0%	30%
6. Surface Tension	0%	30%
7. Viscosity	0%	30%
8. Thermal Conductivity	0%	30%
9. Heat of Formation	0%	30%
10. Gibb's Free Energy of Formation	0%	30%

The compilation and collection activities cover preparation of the manuscript, figures (graphs) and tables for use in the final report.

The property data coverage in the final report will include the following chemical materials important in the processing and production operations for silicon of semiconductor and solar cell grade quality: silane, dichlorosilane, trichlorosilane, silicon tetrachloride, silicon tetrafluoride and silicon.

II. CHEMICAL ENGINEERING ANALYSIS

Chemical engineering analysis of the DCS process (dichlorosilane) - Case A was continued. The approach for the DCS process - which is involved in the Hemlock Semiconductor Corporation program for polysilicon - is based on performing initial analysis of the dichlorosilane (DCS) production. Upon completion of the chemical engineering analysis of the DCS production, then analysis of polysilicon production from the DCS will be performed. Experimental data and results from the Hemlock Semiconductor Corporation program using DCS as the feedstock will be used in the polysilicon production analysis.

For the DCS process, status and progress are summarized below for the primary chemical engineering analysis activities:

	<u>Prior</u>	<u>Current</u>
1. Base Case Conditions	65%	100%
2. Reaction Chemistry	65%	100%
3. Process Flow Diagram	60%	100%
4. Material Balance	50%	100%
5. Energy Balance	40%	100%
6. Property Data	30%	100%
7. Equipment Design	10%	100%
8. List of Major Equipment	5%	100%
9. Production Labor	0%	100%

Case A of the DCS process involves a final distillation column added at the end of the process to separate potential light components (silane, monochlorosilane, diborane, etc.) from the desired dichlorosilane (DCS) product. This distillation column helps insure the purity of DCS and helps reduce potential dust formation chlorosilanes (SiH_4 , SiH_3Cl) in the feed to the chemical vapor deposition reactor for polysilicon production.

In the UCC silane process (Union Carbide Corporation) for silicon, a final distillation is used to remove the boron impurity from the silicon feed source material (silane). In that process, the boron impurity is removed as diborane (B_2H_6)

in the final distillation. The present Case A (DCS process) includes a final distillation for the removal of boron impurity in the form of diborane (B_2H_6).

A process design was performed to obtain data for a cost analysis of a plant to produce dichlorosilane (DCS) as a silicon source material for polysilicon production. 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:

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

TABLE II-1 CHEMICAL ENGINEERING ANALYSES:
PRELIMINARY PROCESS DESIGN ACTIVITIES FOR DCS PROCESS - CASE A

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

Figure II-1 Process Flowsheet for DCS Process - Case A

TABLE II-2

BASE CASE CONDITIONS FOR DCS PROCESS - CASE A

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
 - H₂/Cl₂ ration about 2.8
 - 30% conversion of SiCl₄ to SiHCl₃
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 (B₂H₆, 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 II-3

REACTION CHEMISTRY FOR DCS PROCESS - CASE A

1. Hydrochlorination Reaction 2. Redistribution Reaction 3. Waste Treatment (representative - overall) 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 II-4

RAW MATERIAL REQUIREMENTS FOR DCS PROCESS - CASE A

	<u>Raw Material</u>	<u>Requirements lb/hr</u>	<u>lb/kg of DCS</u>
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 II-5

UTILITY REQUIREMENTS FOR DCS PROCESS - CASE A

<u>Utilities/Function</u>	<u>Total Requirements</u>	<u>Requirements per Kg of DCS</u>
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 x 10 ⁶ MM Btu/hr)	10.6 gal/hr	.008 gal
	44.0 gal/hr	.034 gal

TABLE II-6

LIST OF MAJOR PROCESS EQUIPMENT
FOR DCS PROCESS-CASE A

<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material of Construction</u>
<u>Reactors</u>				
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 Com-buster	To incinerate waste vapors	25 SCFM Vapor/Combustion	3' x 3' x 9' 14.7 psia	CS/Brick
<u>Distillation Columns</u>				
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 II-6 (continued)

<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material of Construction</u>
<u>Tanks & Bins</u>				
9. 3-01 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 Settling 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 II-6 (continued)

	<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material Construction</u>
20.	D-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	Tc prepare lime solution	8 hr. storage, Vertical, open top	5' diam. x 9.5'	CS
22.	T-13 Waste Filtrate Storage Tank	Tc store waste filtrate	4 hr. storage, vertical	5' diam. x 8'	CS
<u>Heaters & Heat Exchangers</u>					
23.	H-01 Crude TCS Condenser	Tc condense chlorosilanes	8.4MM Btu/Hr. Shell-Tube H.E.	1211 ft ² , 515 psia	316SS
12 24.	H-02 H ₂ Gas Pre-heater	Tc 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	Tc 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	Tc 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 II-6 (continued)

	<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material of Construction</u>
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	282 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 Super-heater	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
<u>Compressors and Pumps</u>					
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 II-6 (continued)

	<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material of Construction</u>
	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	Pneumatic 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 Hydro-chlorination reactor	42.2 gpm centrifugal	15bhp, discharge press. 500 psia	CS
14	46. P-06 DCS Reflux Pump	Pumping DCS for D-03 reflux and feed to D-04	6.5 gpm centrifugal	4bhp, discharge press. 355 psia	316SS
	47. P-08 DCS Purification Discharge Pump	To withdraw impurities from DCS Purification unit	2.6 gpm centrifugal	4 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 II-6 (continued)

<u>Equipment</u>	<u>Function</u>	<u>Duty/Type</u>	<u>Size</u>	<u>Material of Construction</u>
<u>Miscellaneous</u>				
52. -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 II-7

PRODUCTION LABOR REQUIREMENTS FOR DCS PROCESS - CASE A

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

III. ECONOMIC ANALYSES

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 III-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\$/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 III-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\$/kg of DCS (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 III-3
• Process Design Inputs.....	Table III-4
• Base Case Conditions.....	Table III-5
• Raw Material Cost.....	Table III-6
• Utility Cost.....	Table III-7
• Major Process Equipment Cost.....	Table III-8
• Production Labor Cost.....	Table III-9
• Plant Investment.....	Table III-10
• Total Product Cost.....	Table III-11

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

TABLE III-1

ESTIMATION OF PRODUCT COST FOR DCS PROCESS - CASE A

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

TABLE III-2

COST AND PROFITABILITY ANALYSIS SUMMARY FOR DCS PROCESS - CASE A

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	<u>0.83 Mega</u>	<u>1.16 Mega</u>
(15%) Total	6.36 Mega	8.90 Mega
	(1975 dollars)	(1980 dollars)

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

	<u>Sales Price</u> <u>\$/Kg of DCS</u> <u>(1975 dollars)</u>	<u>Sales Price</u> <u>\$/Kg of DCS</u> <u>(1980 dollars)</u>
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)

	<u>Sales Price</u> <u>\$/Kg of DCS</u> <u>(1975 dollars)</u>	<u>Sales Price</u> <u>\$/Kg of DCS</u> <u>(1980 dollars)</u>
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.

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

Prel. Process Economic Activity		Status	Prel. Process Economic Activity		Status
1.	Process Design Inputs	0	6.	Production Labor Costs	0
1.	Raw Material Requirements	0	1.	Base Cost Per Man Hour	0
2.	Utility Requirements	0	2.	Cost/Kg Silicon Per Area	0
3.	Equipment List	0	3.	Total Cost/Kg Silicon	0
4.	Labor Requirements	0			
2.	Specify Base Case Conditions	0	7.	Estimation of Plant Investment	0
1.	Base Year for Costs	0	1.	Battery Limits Direct Costs	0
2.	Appropriate Indices for Costs	0	2.	Other Direct Costs	0
3.	Additional	0	3.	Indirect Costs	0
			4.	Contingency	0
3.	Raw Material Costs	0	5.	Total Plant Investment (Fixed Capital)	0
1.	Base Cost/Lb. of Material	0			
2.	Material Cost/Kg of Silicon	0	8.	Estimation of Total Product Cost	0
3.	Total Cost/Kg of Silicon	0	1.	Direct Manufacturing Cost	0
			2.	Indirect Manufacturing Cost	0
4.	Utility Costs	0	3.	Plant Overhead	0
1.	Base Cost for Each Utility	0	4.	By-Product Credit	0
2.	Utility Cost/Kg of Silicon	0	5.	General Expenses	0
3.	Total Cost/Kg of Silicon	0	6.	Total Cost of Product	0
5.	Major Process Equipment Costs	0			
1.	Individual Equipment Cost	0			
2.	Cost Index Adjustment	0			

0 Plan

0 In Progress

0 Complete

TABLE III-4

PROCESS DESIGN INPUTS FOR DCS 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
 - 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 III-5
BASE CASE CONDITION FOR DCS 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 = 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 III-6

RAW MATERIAL COST FOR DCS PROCESS - CASE A

<u>Raw Material</u>	<u>Requirement lb/kg of DCS</u>	<u>\$/lb of material</u>	<u>Cost \$/kg of DCS</u>
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	<u>0.0036</u>
		TOTAL	0.5509 (1975 dollars)
			<u>x 1.4</u> inflation
			0.7713 (1980 dollars)

TABLE III-7

UTILITY COST FOR DCS PROCESS - CASE A

<u>Utility</u>	<u>Requirement/kg of DCS</u>	<u>Cost of Utility</u>	<u>Cost \$/kg of DCS</u>
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	<u>0.00662</u>
		TOTAL	0.04005 (1975 dollars)
			<u>x 1.4</u> inflation
			0.05607 (1980 dollars)

TABLE III-8

PURCHASED COST OF MAJOR PROCESS EQUIPMENT
FOR DCS PROCESS - CASE A

	<u>Equipment</u>	<u>Purchased Cost, \$1000</u>
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 III-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 Pre- paration Tank	0.9
22.	T-13 Waste Filtrate Storage Tank	0.9
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 III-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-02 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	<u>1.3</u>
		891.6 (1975 dollars)
		x 1.4 inflation
		<u>1,248.2</u> (1980 dollars)

TABLE III-9

PRODUCTION LABOR COST FOR DCS PROCESS - CASE A

<u>Section</u>	<u>Labor man-hr/Kg DCS</u>	<u>Labor \$/man-hr</u>	<u>Cost \$/Kg DCS</u>
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 III-10

ESTIMATION OF PLANT INVESTMENT FOR DCS PROCESS - CASE A

	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	<u>1,275.9</u>
7. FIXED CAPITAL INVESTMENT FOR PLANT, 5 + 6	5,528.8 (1975 dollars)
	x 1.4 inflation
8. WORKING CAPITAL INVESTMENT FOR PLANT, % OF 6	<u>7,740.3</u> (1980 dollars)
9. TOTAL PLANT INVESTMENT, 7 + 8	

TABLE III-11

ESTIMATION OF TOTAL PRODUCT COST FOR DCS PROCESS - CASE A

	<u>\$/KG of DCS</u>
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	<u>0.0241</u>
6. Total Cost of Product, 4a + 5	0.9230 (1975 dollars)
	<u>x 1.4 inflation</u>
	1.2922 (1980 dollars)

IV. SUMMARY - CONCLUSIONS

The following summary-conclusions are made as a result of progress during this reporting period.

1. Task 1

Analyses of process system properties were continued for chemical materials important in the production of silicon including compilation and collection activities of the property data for use in the final report. Progress and status are reported for critical constants, vapor pressure, heat of vaporization, heat capacity, density, surface tension, viscosity, thermal conductivity, heat of formation and Gibb's free energy of formation. Compilation and collection activities are about 30% complete covering preparation of the manuscript, figures (graphs) and tables for the final report.

2. Task 2

Major efforts in chemical engineering analysis centered on the DCS process - Case A which involves production of dichlorosilane (DCS) as a silicon source material for polysilicon production in the Hemlock Semiconductor Corporation program. The preliminary process design of a plant to produce DCS was completed including process flowsheet (100%), base case conditions (100%), reaction chemistry (100%), raw materials (100%), utilities (100%), major process equipment (100%) and production labor (100%). The process design package was forwarded for economic analysis.

3. Task 3

The cost analysis of the DCS process - Case A was completed during this reporting period. The results for dichlorosilane (DCS) indicated a total product cost without profit of 1.29\$/kg (1980 dollars). This product cost without profit includes direct manufacturing cost, indirect manufacturing cost, plant overhead and general expenses. The sales price of DCS at 15% DCF rate of return on investment is 1.47\$/kg (1980 dollars). Additional results are reported for sales price of dichlorosilane at various profitability levels as measured by ROI (return on original investment) and DCF (discounted cash flow rate of return).

V. PLANS

Major efforts will be devoted to compilation and collection activities for the final report covering preparation of the manuscript, figures (graphs and flowsheets) and tables. The final report will cover process system properties, chemical engineering and economic analyses of chemical materials and processes important to the production of silicon.

MILESTONE CHART

TASK	1975			1976												1977-1979												1980													
	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A						
1. Analyses of Process																																									
<u>System Properties</u>																																									
1. Prel. Data Collection																																									
2. Data Analysis																																									
3. Estimation Methods																																									
4. Exp.-Corr. Activities																																									
5. Prel. Prop. Values																																									
2. Chemical Engineering																																									
<u>Analyses</u>																																									
1. Prel. Process Flow Diag.																																									
2. Reaction Chemistry																																									
3. Kinetic Rate Data																																									
4. Major Equip. Req.																																									
5. Chem. Equil.-Exp. Act.																																									
6. Process Comparison																																									
3. Economic Analyses																																									
1. Cap. Invest. Est.																																									
2. Raw Materials																																									
3. Utilities																																									
4. Direct Manuf. Costs																																									
5. Indirect Costs																																									
6. Total Cost																																									
7. Process Comparison																																									
Final Report																																									

PROCESS FEASIBILITY STUDY IN
SUPPORT OF SILICON MATERIAL TASK I

JPL Contract No. 954343