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PROCESS FEASIBILITY STUDY IN SUPPORT
OF SILICON MATERIAL TASK I

Quarterly Technical Progress Report II

C. L. Yaws

April 1976

Work Performed Under Contract No. JPL 954343

Department of Chemical Engineering
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Beaumont, Texas

MASTER

ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
Division of Solar Energy

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Carl L. Yaws

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ABSTRACT

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

In Task 1, preliminary data collection is very near completion for the silicon source materials - silane (SiH_4), silicon tetrachloride (SiCl_4) and silicon tetraiodide (SiI_4) - which are associated with the silane, Zn/SiCl_4 and H_2/SiI_4 processes under consideration. Major effort was initiated on the silicon source materials - silicon tetrafluoride (SiF_4) and silicon difluoride (SiF_2) - for the transport process.

In addition, preliminary results for the critical constants and physical properties of silane (SiH_4) were tabulated. The sole data source is based on work performed approximately sixty-five years ago in 1911. The fraction boiling at -116°C was used. Since the boiling point of silane is generally accepted as -112°C , the values for critical temperature (T_c) and pressure (P_c) are subject to question. Data for the remaining critical constants-volume (V_c), compressibility factor (Z_c) and density (ρ_c) - are apparently not available.

For Task 2, initial background technical information exchange was accomplished on the following processes in the task integration meeting and subsequent discussions: Zn/SiCl_4 (Battelle); H_2/SiI_4 (Battelle); silane (Union Carbide); transport (Motorola); induction plasma (Texas Instruments); arc furnace (Dow Corning) and SiF_4 reduction (Stanford).

Several base case conditions including a plant size of 1000 metric tons/yr. were tentatively suggested and selected. Three such plants would provide the required 3000 metric tons/yr. of solar cell grade silicon.

In Task 3, procurement of data sources for numerous equipment types was accomplished for use in economic analysis. A review of methods for estimating capital investment was also initiated. Three methods were identified: (1) Ratio Factor Method, (2) Lang Factor Method and (3) Turnover Ratio Method. The Ratio Factor Method appears best suited for application to the solar cell grade silicon processes. The method is based on capital investment (fixed, working and total) as a percentage of the cost of major process equipment associated with the process under consideration.

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MILESTONE CHART	

I. PROCESS SYSTEM PROPERTIES ANALYSES (TASK 1)

Preliminary data collection activities were continued during this reporting period on major physical, transport and thermodynamic properties essential to assessment of the alternate processes for solar cell grade silicon. Primary efforts were devoted to the silicon source materials associated with the silane (SiH_4), Zn/SiCl_4 and H_2/SiI_4 (or SiI_4 dissociation) processes.

Preliminary data collection is very near completion for the silicon source materials - silane (SiH_4), silicon tetrachloride (SiCl_4), and silicon tetraiodide (SiI_4) - which are associated with the silane, Zn/SiCl_4 and H_2/SiI_4 (or SiI_4 dissociation) processes. Data source procurement from the majority of the domestic sources has been accomplished. Requests for the same have been issued for the foreign sources (Russian, Japan, German, etc.).

Major effort was initiated on the silicon source materials - silicon tetrafluoride (SiF_4) and silicon difluoride (SiF_2) - which are associated with the transport process.

The data analysis activity was initiated in accordance with the program schedule. Preliminary data analysis results are shown in Table I for silane (SiH_4), silicon tetrachloride (SiCl_4) and silicon tetraiodide (SiI_4). The preliminary listing identifies both (a) those properties for which few data sources are available and (b) those properties for which no data source is available.

Compilation of data sources in accordance with the coding system is in progress for the silicon source materials. Compilation results for Code A (silane, SiH_4), B (silicon tetrachloride, SiCl_4), and C (silicon tetraiodide, SiI_4) are presented in the Appendix.

For the silane process, data analysis centered on critical constants for silane (SiH_4). Preliminary results are given in Table II. Experimental data for the critical temperature and pressure of silane are available (A2, A15, A20, A22, A23, A25, A27, A29, A45, A49, A50, A51). However, all sources cite Adwentowski (A51) who did his work approximately sixty-five years ago in 1911. Adwentowski prepared the sample from magnesium silicide and used the fraction boiling at -116°C . Since the boiling point of silane is generally accepted at -111.9°C , these results may not be completely reliable and are questionable. No data are available for the remaining critical constants--critical volume, compressibility factor and density.

TABLE I PRELIMINARY DATA ANALYSIS FOR PROCESS SYSTEM PROPERTIES - DATA SOURCE IDENTIFICATION AND AVAILABILITY

PROPERTY	SILANE <u>SiH₄</u>	SILICON TETRACHLORIDE <u>SiCl₄</u>	SILICON TETRAIODIDE <u>SiI₄</u>
1. CRITICAL CONSTANTS	0	0	0
.1 CRITICAL TEMP. (T _C)	0	0	0
.2 CRITICAL PRESSURE (P _C)	0	0	0
.3 CRITICAL VOLUME (V _C)	0	0	0
.4 CRITICAL COMPRESSIBILITY FACTOR (Z _C)	0	0	0
2. VAPOR PRESSURE (P _V)	0	0	0
3. HEAT OF VAPORIZATION (ΔH _V)	0	0	0
4. HEAT CAPACITY (C _P)	0	0	0
.1 GAS	0	0	0
.2 LIQUID	0	0	0
5. DENSITY (ρ)	0	0	0
6. VISCOSITY (μ)	0	0	0
.1 GAS	0	0	0
.2 LIQUID	0	0	0
7. SURFACE TENSION (σ)	0	0	0
8. THERMAL CONDUCTIVITY (K)	0	0	0
.1 GAS	0	0	0
.2 LIQUID	0	0	0
9. HEAT OF FORMATION (ΔH _f)	0	0	0
10. FREE ENERGY OF FORMATION (ΔG _f)	0	0	0

CODE

0 ~ NO DATA SOURCE AVAILABLE

0 ~ FEW DATA SOURCES AVAILABLE

0 ~ SEVERAL DATA SOURCES AVAILABLE

TABLE II PRELIMINARY DATA ANALYSIS - CRITICAL CONSTANTS AND PHYSICAL PROPERTIES OF SILANE, SiH_4

Identification	Silane SiH_4
State (std. cond.)	gas (colorless)
Molecular Weight, M	32.12
Boiling Point, T_b , $^{\circ}\text{C}$	-111.9
Melting Point, T_m , $^{\circ}\text{C}$	-184.7
Critical Temp, T_c , $^{\circ}\text{C}$	-3.5 (Questionable Value)
Critical Pressure, P_c , atm	47.8 (Questionable Value)
Critical Volume, V_c , $\text{cm}^3/\text{gr mol}$	--
Critical Compressibility Factor, Z_c	--
Critical Density, ρ_c , gr/cm^3	--

II. CHEMICAL ENGINEERING ANALYSES (TASK 2)

During this reporting period, chemical engineering analyses were continued in accordance with the program schedule.

Initial background technical information exchange was accomplished with individual contractors at the task integration meeting and in subsequent preliminary process discussions. This included progress, status and plans for the following processes under consideration for solar cell grade silicon:

1. Zn/SiCl₄ Process (Battelle)
2. H₂/SiI₄ (or SiI₄ Dissoc.) Process (Battelle)
3. Silane Process (Union Carbide)
4. Transport Process (Motorola)
5. Induction Plasma Process (Texas Instruments)
6. Arc Furnace Process (Dow Corning)
7. SiF₄ Reduction Process (Stanford)

Additional technical information exchange is anticipated in the next several quarters.

In the work session portion of the task integration meeting, the following base case conditions were suggested for use in the chemical engineering analysis of a plant to produce solar cell grade silicon:

1. Plant Size
 - a) 1000 metric tons/year
 - b) metric ton = 2205 lb
2. Cost Index
 - a) base capital equipment cost on Jan. 1975 cost index value
 - b) Jan. 1975 cost index value = 430
3. Operating Ratio
 - a) 80-85% operating ratio discussed
 - b) operating ratio should probably be selected from the following:

80%	292 days/yr operating
85%	310 days/yr operating
90%	329 days/yr operating
95%	347 days/yr operating

Item 1 (plant size of 1000 metric tons/yr) was suggested by several industrial contractors based on probable company preference for three plant sites to accomplish the overall solar cell grade silicon production requirement of 3000 metric tons/yr.

Technical quarterly progress reports were received from Battelle, Univ. of Penn. - Dow Corning and Union Carbide.

III. ECONOMIC ANALYSES (TASK 3)

The economic analysis activity for application to alternate processes under consideration for solar cell grade silicon was continued.

Procurement of data sources for use in capital investment estimation was accomplished for the process equipment types shown in Table III. The table discloses that partial coverage is available for numerous process equipment types.

In addition, a review was initiated for methods for estimating plant capital investment (fixed, working and total) based on purchased cost of major process equipment. The review focused on adaption of the method for economic analysis of the alternate processes under consideration for production of solar cell grade silicon.

Three capital investment estimation methods which are used in preliminary process design and economic evaluation are discussed as follows:

1. Ratio Factor Method
2. Lang Factor Method
3. Turnover Ratio Method

The Ratio Factor Method (ref. 7) is based on the purchased cost of the major process equipment required for the plant. Table IV presents details of the ratio method for estimation of the capital investment for a chemical process plant. In the tabulation, the items (process equipment; installation; instrumentation and controls; piping; electrical; etc.) required for the plant are expressed as a percentage of the purchased equipment cost. This percentage ratio (ratio factor = item percentage/purchased equipment) permits the estimation of the capital investment. In the first column in the tabulation, the typical range is given from the analysis of a wide spectrum of chemical process plants. The typical range covers plants processing solids; solids and fluids and fluids.

The chemical process plant for the production of solar cell grade silicon will most likely involve processing of both fluids and solids. The last column in the tabulation (Table IV) presents the median percentage for the chemical process plant types. These median percentages are applicable for estimation of capital investment for a plant which involves processing of fluids and processing of solids for the manufacture of the product. The median values are:

	Median (% of E)
Fixed Capital Investment	435
Working Capital Investment	77
Total Capital Investment	512

Where E = purchased equipment cost of major process equipment

TABLE III ECONOMIC ANALYSIS: COST DATA COVERAGE FOR
CAPITAL INVESTMENT ESTIMATION

<u>PROCESS EQUIPMENT TYPE</u>	<u>COST DATA AVAILABILITY</u>	<u>DATA SOURCE PROCUREMENT</u>
1. PUMPS	0	0
2. TANKS AND STORAGE EQUIPMENT	0	0
3. HEAT EXCHANGERS	0	0
4. EVAPORATORS	0	0
5. PROCESS HEATERS	0	0
6. PLATE DISTILLATION TOWERS	0	0
7. PACKED COLUMNS	0	0
8. HIGH PRESSURE EQUIPMENT	0	0
9. JACKETED VESSELS	0	0
10. REACTORS (VARIOUS KINDS)	0	0
11. HOPPERS	0	0
12. MAIN TRANSFORMERS	0	0
13. BOILERS	0	0
14. CRUSHERS	0	0
15. DRYERS	0	0
16. MIXERS	0	0
17. MISCELLANEOUS PROCESS EQUIPMENT	0	0

AVAILABILITY

0 COMPREHENSIVE COVERAGE

0 PARTIAL COVERAGE

0 NO COVERAGE

PROCUREMENT

0 PLAN

0 IN PROGRESS

0 COMPLETED

TABLE IV RATIO FACTOR METHOD FOR ESTIMATION OF CAPITAL INVESTMENT
FOR CHEMICAL PROCESS PLANT

	Typical Range (% of E)	Median (% of E)
1. Purchased Equipment Cost, E	100	100
2. Installation of Purchased Equipment	39-47	43
3. Instrumentation and Controls (Installed)	9-18	13.5
4. Piping (Installed)	16-66	41
5. Electrical (Installed)	10-11	10.5
6. Buildings with Services	18-29	23.5
7. Yard Improvements	10-13	11.5
8. Service Facilities (Installed)	40-70	55
9. Land	6	6
10. Engineering and Supervision	32-33	32.5
11. Construction Expenses	34-41	37.5
12. Contractors Fee	17-21	19
13. Contingency	<u>34-42</u>	<u>38</u>
Fixed Capital Investment	387-483	435
Working Capital Investment	<u>68-86</u>	<u>77</u>
Total Capital Investment	455-569	512

Source: Ref. 7

The Lang Factor Method for capital investment estimation is also based on purchased process equipment cost. Table V presents typical and median values. In general, the total capital investment-estimates from the Lang Factor Method and the Ratio Factor Method just discussed are equivalent (515% vs 512%). However, the Lang Factor Method does not provide detailed percentage of the sub-items (installation; instrumentation and controls; etc.) required for the chemical process plant.

With such detailed percentage factors as provided by the Ratio Factor Method, it is possible to ascertain the influence of the sub-items. For example, suppose a chemical plant with a high degree of automation and control is desired. For this case, the subitem percentage for instrumentation and control may be increased upward (perhaps 2x) to provide the estimated capital costs associated with the high degree of automation for the chemical plant.

The Turnover Ratio Method is sometimes used for rapid order-of-magnitude estimates. The turnover ratio (gross annual sales/fixed capital investment) is approximately 1 for certain processes. However it may range as high as 5. The reciprocal of the ratio method is called the capital ratio.

TABLE V LANG FACTOR METHOD FOR ESTIMATION OF CAPITAL INVESTMENT

	Typical Range (% of E)	Median (% of E)
Purchased Equipment Cost, E	100	100
Fixed Capital Investment	390-480	435
Working Capital Investment	<u>70-90</u>	<u>80</u>
Total Capital Investment	460-570	515

Source: Ref. 7

IV. SUMMARY - CONCLUSIONS

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

1. Task 1

In process system properties, primary data analysis activities were devoted to silicon source materials.

Preliminary data collection is very near completion for the silicon source materials - silane (SiH_4), silicon tetrachloride (SiCl_4) and silicon tetraiodide (SiI_4) - which are associated with the silane, Zn/SiCl_4 and H_2/SiI_4 processes under consideration for solar cell grade silicon. Major effort was initiated on the silicon source materials - silicon tetrafluoride (SiF_4) and silicon difluoride (SiF_2) - for the transport process.

In the silane process, preliminary results for critical constants of silane (SiH_4) were tabulated. The sole data source (A51) for critical temperature and pressure is based on work accomplished approximately sixty-five years ago in 1911. The fraction boiling at -116°C was used. Since the boiling point of silane is generally accepted at -111.9°C , the values are subject to question. No data is available for the remaining critical constants--volume, compressibility factor and density.

Compilation of data sources in accordance with the coding system was accomplished for additional silicon source materials--silicon tetrachloride (SiCl_4) and silicon tetraiodide (SiI_4).

2. Task 2

Initial background technical information exchange was accomplished on the following processes: Zn/SiCl_4 (Battelle); H_2SiI_4 (Battelle); silane (Union Carbide); transport (Motorola); induction plasma (Texas Instruments) and arc furnace (Dow Corning).

Several base case conditions including a plant size of 1000 metric tons/yr. were tentatively suggested and selected. Three such plants would provide the required 3000 metric tons/yr of solar cell grade silicon.

3. Task 3

Procurement of data sources for numerous process equipment types was accomplished for use in the economic analysis activity.

A review of methods for estimating plant capital investment was initiated. The review focused on adaption of the method for economic analysis of the alternate processes for solar cell grade silicon.

Three capital investment estimation methods were identified for use in preliminary process design and economic evaluation: (1) Ratio Factor Method; (2) Lang Factor Method, and (3) Turnover Ratio Method.

The Ratio Factor Method appears best suited and amenable for application to the alternate solar cell grade silicon process. The method is based on capital investment as a percentage of the purchased process equipment cost.

V. PLANS

Plans for the next reporting period are summarized below.

1. Task 1

Conduct additional data analysis activities for process system properties.

Continue data source efforts--identification, procurement and compilation--for the additional silicon source material--silicon tetrafluoride (SiF_4).

2. Task 2

Conduct process discussions as required on alternate processes for solar cell grade silicon.

Screen technical progress reports as received for information relative to chemical engineering analysis.

3. Task 3

Continue economic analysis activities.

Initiate review of methods for estimation of total product cost. Focus on adaption of method to processes for solar cell grade silicon.

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Appendix A

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Appendix C

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PROCESS FEASIBILITY STUDY IN
SUPPORT OF SILICON MATERIAL TASK I