June 22, 1992

U. S. Department of Energy
Pittsburgh Energy Technology Center
Mail Stop 922-H
P. O. Box 10940
Pittsburgh, PA 15236

Attention: Mr. Swenam Lee
Project Manager

Subject: D.O.E. Coal Liquefaction
Base Line Design and System Analysis
Contract No. DE-AC22 90PC89857
Bechtel Job No. 20952
Quarterly Status Report
Letter No. BLD-101

Dear Mr. Lee:

Attached for your information are three copies of the subject Quarterly Status Report covering the December 23, 1991 through March 15, 1992 reporting period. Copies to other members, as required by the contract are separately and directly transmitted.

Please note that all information contained herein should be considered preliminary pending issue of the final tasks reports.

This report contains confidential information which, as agreed, has been segregated in the appendix of this report.

If you have any questions or comments on this Quarterly Status Report please contact me.

Sincerely yours,

Sam N. Habash
Project Manager

Attachment:

cc: Martin Byrnes, DOE/PETC
    Robert Hamilton, DOE/PETC
    A. B. Schachtenschneider, AMOCO File
    Gilbert V. McGurl, DOE/PETC
    Joanne Wastek, DOE/PETC
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DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
1. INTRODUCTION

Effective May 16, 1990, Bechtel with Amoco as subcontractor, initiated a study to develop a computer model for a base line direct coal liquefaction design for the U.S. Department of Energy's (DOE) Pittsburgh Energy Technology Center (PETC). The project was initially for a duration of 18 months with an approved budget of $2 MM. Later, the project was extended to mid-May 1992. This study is under DOE contract No. DE-AC22 90PC89857.

The primary objective of the study is to develop a computer model for a base line direct coal liquefaction design based on two stage direct coupled catalytic reactors. This primary objective is to be accomplished by completing the following:

- A base line design based on previous DOE/PETC results from Wilsonville pilot plant and other engineering evaluations
- A cost estimate and economic analysis
- A computer model incorporating the above two steps over a wide range of capacities and selected process alternatives
- A comprehensive training program for DOE/PETC Staff to understand and use the computer model
- A thorough documentation of all underlying assumptions for baseline economics, and
- A user manual and training material which will facilitate updating of the model in the future

The progress made during any particular quarter is published in a quarterly report following the duration of the quarter. The report consists of the following four sections:

- Introduction
- Summary
- Technical Progress Report (By Tasks)
- Key Personnel Staffing Report.
Introduction (Continued)

Any confidential information will be presented in the quarterly report as a separate section under the heading "confidential". As agreed upon by DOE/PETC, information included in the confidential section will be treated confidential by DOE/PETC and its contractors.

This report is Bechtel's seventh quarterly progress report and covers the period of December 23, 1991 through March 15, 1992.
2. SUMMARY

Effective May 16, 1990, Bechtel initiated this study, with Amoco as subcontractor, as an assignment from the U.S. Department of Energy (DOE)'s Pittsburgh Energy Technology Center (PETC). The objective of the study is to develop a computer model for a baseline direct coal liquefaction design based on two stage direct coupled catalytic reactors. The study was for a period of 18 months which was extended later to mid-May, 1992 with an approved total budget of approximately $2MM.

This is Bechtel's sixth quarterly progress report and covers the period (as requested and approved by DOE/PETC) of December 23, 1991 through March 15, 1992. This reporting period was previously covered by three already published monthly status reports.

The report contains accomplishments made during this time period in all the Tasks scheduled for the period i.e., Tasks I through VI. As per schedule, the major focus, however, was on Task II, III, IV and V. Therefore, the accomplishments included in this report are predominantly for these four tasks.

The accomplishments are presented in the report on Task by Task basis for all the Tasks covered during this reporting period.

In Task I (which defines the project) the Project Management Plan Draft Report was completed and subsequently updated incorporating the comments and suggestions of DOE/PETC and their contractors. The final version was sent to DOE/PETC for their approval and subsequently published in August, 1990. The approved copy was the deliverable for the Task.

Project Management Plan report covers the overall scope of work, the methodology of managing the cost and schedule of the project (configuration management), program administration, the deliverables during various phases of work and the definition of the baseline configuration.

Task II

- During this reporting period Volume III of this task was issued as a draft as well as a final task/topical report.
Task III

- Preliminary capital cost estimates for all the options as well as economics for various scenarios have been completed for DOE/PETC's review during DOE/PETC/Bechtel/Amoco review meeting on February 24-25, 1992 at Naperville.
- The operating cost estimates and baseline case economics are being developed.
- Based on the DOE/PETC/Bechtel/Amoco review meeting on February 24-25, 1992 capital cost estimates for the baseline design as well as all seven options have been initiated for two different scenarios. These scenarios are for: 1) the "First Plant" and, 2) "Nth Plant". The cost estimates will be carried out for each ISBL plant and for the entire complex.

Task IV

- This task was completed and final report issued the first week in October, 1991.

Task V

- Continued validation of the model versus the final release of the Task II report. All baseline plants except Plant 39, phenol recovery plant, have been tuned to match the baseline design in a stand-alone mode. Progress is being made on integrating the system in a combined model. Changes reflecting the outcome of the February DOE/PETC/Bechtel/Amoco review meeting need to be incorporated.
- The ASPEN based kinetic model is being tuned to match the baseline design. A first draft of the documentation has been prepared.
- A first draft of the documentation of the FORTRAN block models for the Task 5 report has been completed.
- Finalization of the Lotus spreadsheet economic model is awaiting comments following discussion at the February DOE/PETC/Bechtel/Amoco review meeting. Documentation has been prepared.
- As a part of SSI's subcontract, the subroutines for retrieving and loading pseudocomponent properties from the internal ASPEN storage for transfer from one process module to another are being developed. Integration of the subroutines into various FORTRAN block models has not yet been started.
Task VI

• The ASPEN training course is scheduled for the week of March 23, 1992 at the DOE/PETC facilities in Pittsburgh.

• A first draft of the documentation of Task 6, the training manual, is being prepared. This will be used for the proposed DOE training session.
3. TECHNICAL PROGRESS (BY TASKS)

In order to carry out this Study efficiently, the Study has been divided in seven major tasks. Task I defines the project. Task II develops the baseline design. Task III develops the capital, operating and maintenance costs. Task IV develops the mathematical model necessary for the process computer simulation model. Task V develops and verifies the process simulation model. Task VI documents the process simulation model and training. Task VII is a level of effort task for project management, technical coordination and other miscellaneous support functions.

During this reporting period (December 23, 1991 through March 15, 1992) several accomplishments were made in Tasks II, III, IV and VI. These accomplishments are included in this report task by task.

Task I was completed during the first quarterly reporting period. The accomplishment of Task I was documented in the Project Management Plan published in August, 1990. It was also presented in the first quarterly report, covering the period of May 16, 1990 through August 19, 1990).
3.1 TASK I

Task I defines the scope and the methodology of accomplishing the project. It sets the objectives of the project and defines the paths to accomplish those objectives.

As mentioned earlier in Section 3, Task I was completed during the first quarterly reporting period and accomplishments were documented in the Project Management Plan issued in August, 1990.

The Project Management Plan report is comprised of the following 9 sections:

- Executive Summary
- Background/Introduction
- Study Objective
- Overall Scope Of Work
- Configurational Management
- Program Administration
- Deliverables
- Baseline Configuration
- Appendix/Project Procedure Booklet
- List Of Contents

The report completing Task 1 was published on time schedule. Detailed accomplishments of Task I were included in the first quarterly report (May 16, 1990 through August 19, 1990) of the project.
3.2 TASK II

Task II concerns the development of the baseline design of the liquefaction facility. This part of the study includes the acquisition of process licensors information, incorporation of various processing options into the design, and developing the design of the on-site processing units and offsite facilities (including storage and loading, utilities, and waste handling).

In this task certain plants are handled as packaged plants (or blocks) with an overall heat and material balance only.

3.2.1 STATUS UPDATE

The final Topical/Task report for task II is divided into three volumes. Volumes I and II contain the information on the baseline design while volume III covers the options (alternates). Volumes I and II of the report were published during the quarter of September 16, 1991 through December 22, 1991 reporting period.

During this reporting period, Volume III of the report, both draft and the final version were published. The table of contents of Volume III is included in this report. As one may notice the report starts with section 43 which pertains to the selection methodology for various options and the deliverables. In addition, there are seven more sections (sections 44 through 50) for the seven selected options. Information included in each of these sections are:

- Design basis, criteria and considerations
- Process description/process flow diagram for the directly affected plant
- Material balance for the directly affected plant
- Utility summary for the directly affected plant
- Overall impact
- Overall plant configuration and overall material balance
- Overall utility summary
- Overall water flow distribution
- Overall hydrogen flow distribution
# TASK II REPORT

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**VOLUME III, SECTIONS 43 - 50**

### 43. Definition of Options To Base Line Design

- 43.1 Methodology For Selection
- 43.2 Deliverables

### 44. Option 1 (Liquefaction Feed Coal Cleaning by Heavy Media Separation)

- 44.1 Design Basis, Criteria and Considerations
- 44.2 Process Description/Process Flow Diagram for the Directly Affected Plant
- 44.3 Material Balance for the Directly Affected Plant
- 44.4 Utility Summary for the Directly Affected Plant
- 44.5 Overall Impact
- 44.5.1 Overall Plant Configuration and Overall Material Balance
- 44.5.2 Overall Utility Summary
- 44.5.3 Overall Water Flow Distribution
- 44.5.4 Overall Hydrogen Flow Distribution

### 45. Option 2 (Liquefaction Feed Coal Cleaning by Spherical Agglomeration)

- 45.1 Design Basis, Criteria and Considerations
- 45.2 Process Description/Process Flow Diagram for the Directly Affected Plant
- 45.3 Material Balance for the Directly Affected Plant
- 45.4 Utility Summary for the Directly Affected Plant
- 45.5 Overall Impact
- 45.5.1 Overall Plant Configuration and Overall Material Balance
- 45.5.2 Overall Utility Summary
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### 46. Option 3 (Thermal-Catalytic Liquefaction Reactor Configuration)

- 46.1 Design Basis, Criteria and Considerations
- 46.2 Process Description/Process Flow Diagram for the Directly Affected Plant
- 46.3 Material Balance for the Directly Affected Plant
- 46.4 Utility Summary for the Directly Affected Plant
- 46.5 Overall Impact
- 46.5.1 Overall Plant Configuration and Overall Material Balance
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47. Option 4 (Catalytic-Catalytic Reactor Configuration With Vent Gas Separation Option)

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48. Option 5 (Fluid Coking of Vacuum Bottoms)

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49. Option 6 (Steam Reforming of Natural Gas Plus FBC Unit for Hydrogen Production)
## 50. Option 7 (Naphtha Reforming)

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3.3 TASK III

Task III concerns the development of the cost estimate and economics for the base-line design and the alternates for the coal liquefaction facility. This part of the study includes the compilation of equipment and utilities summaries, development of scaling factors for equipment sizes and plant costs, and development of the estimates for capital cost, working capital, and owner's costs. Work to perform the economic analyses includes the workup of the manpower requirements and operating costs for the baseline design and for the options and the completion of sensitivity studies.

In this task plants are handled as packaged plants or blocks for the purpose of capital investment, and operating costs as well as overall capacity scale-up.
3.3.1 Capital Cost Estimates for Options

During this reporting period the methodology to develop the capital cost estimates was completed. This was followed by developing the preliminary cost estimates for each option. The preliminary results on capital cost thus estimated are included in the confidential section of the report, whereas the methodology utilized for the capital cost estimates for various options is presented here:

**CAPITAL COST OF OPTIONS**

Capital cost for each option was estimated by:

- Estimating the capital costs for the directly affected plant.
- Adjusting the capital costs for the indirectly affected plant
  - Capital costs adjustment for each of the indirectly affected plant was achieved by scaling the base case cost based on throughput
- Base case capital cost for each ISBL plant was estimated by utilizing following steps:
  1) Calculate field costs by summing up the estimated costs of five components i.e., major equipment, bulk material, subcontracts, direct labor and distributables.
  2) Allocate capital costs for OSBL plants to each ISBL plant capital cost.
  3) Include home office, fee and contingency to the adjusted costs as obtained in step 2 to calculate the installed plant cost.
3.3.2 Economic Scenarios

Several economic scenarios to improve the overall economics were developed during this reporting period and presented to DOE/PETC during February 24 and 25, 1992 project review meeting at Naperville, Illinois. These are shown below:

VARIOUS SCENARIOS TO IMPROVE THE OVERALL ECONOMICS

- Base Case Economics appear to be unattractive primarily because of the inherent conservative design basis of the baseline.

- The various scenarios presented below as Cases A through G are intended to relax some of these conservative constraints.

- Capital Cost Impacts for Cases A through D are estimated. In addition three other scenarios (Cases E through G) are presented as a "food for thought" for potential future study and considered to have favorable capital cost impact.

Case A:

Base case without "not so critical" sparing

Case B:

Case A with improved design basis

Case C:

Case B with hydrogen by natural gas reforming

Case D:

Case C with Nth plant scenario
VARIOUS SCENARIOS TO IMPROVE THE OVERALL ECONOMICS
(continued)

"Food for Thought"

Case E:

Case D with optimum product valuation

Case F:

Additional process related capital cost reduction Scenario

Case G:

Additional site related capital cost reduction scenario
3.3.3 First Plant and Nth Plant Concepts

During February 24 and 25, 1992 DOE/PETC project review meeting discussion was carried out on the "First Plant" and "Nth Plant" concepts. These concepts are described below:

3.3.3.1 First & Nth Plant Concepts

For any developing technology where the first commercial plant has not been built, there is a period of time certain items are initially assumed and later revised downward as the technology's commercial history is established. Such items are:

1. Design Basis including scale-up considerations (from the plant capacity at which the technology was proven to the capacity of the commercial plant).

2. Assumed design overcapacity factors which take the form of sparing of whole production trains. These over capacity factors have a direct impact on the onstream factor.

3. Project Schedule

The First plant concept is thus self-explanatory. It refers to the first commercial plant with a degree of over design to meet the name plate capacities and product specifications.

The period of time between the first commercial plant and the plant at which the technology commercial maturity is normally designated as N years. Thus the Nth plant is that commercial plant built N years after the first commercial plant for which the technology basis, plant design and operation are well known.

The focus of this task (Task III) is to define and develop the Nth plant economics, as requested by DOE.

The Nth plant economics are defined as the economics of the Nth plant which has the following characteristics:

1. requires lowest reasonable plant cost contingency;

2. contains no spare trains;

3. incurs the lowest reasonable engineering cost;

4. requires the lowest possible project schedule to erect and start-up;

5. technology has matured to the point that the Nth plant overall stream factor of the complex remains the same as that of the First plant.

Cost estimates following these concepts were initiated during this reporting period
following the above mentioned meeting.

3.4 TASK IV

Task IV concerns the development of the mathematical algorithms and models for equipment sizing, scale-up, costing, and train duplication for incorporation into the ASPEN/SP process simulation model being developed in Task V.

3.4.1 Status of Task IV

The final topical/task report for Task IV was published in October 1991.
3.5  TASK V

Task V concerns the development of the ASPEN process simulation model of the baseline design. The model will produce complete heat and material balances, elemental balances around each plant and the entire process complex, a major equipment list and outline specifications for Plant 2, utility requirements, capital cost for all plants, and a discounted cash flow economic model for the total complex. The model will be suitable for studying technology advances and options in a case study approach. The model will not include optimization capabilities.

During this reporting period several accomplishments were made in this task. These accomplishments are listed below.

- Continued validation of the model versus the final release of the Task II report. All baseline plants except Plant 39, phenol recovery plant, have been tuned to match the baseline design in a stand-alone mode. Progress is being made on integrating the system in a combined model. Changes reflecting the outcome of the February DOE/PETC/Bechtel/Amoco review meeting need to be incorporated.

- The ASPEN based kinetic model is being tuned to match the baseline design. A first draft of the documentation has been prepared.

- A first draft of the documentation of the FORTRAN block models for the Task 5 report has been completed.

- Finalization of the Lotus spreadsheet economic model is awaiting comments following discussion at the February DOE/PETC/Bechtel/Amoco review meeting. Documentation has been prepared.

- As a part of SSI's subcontract, the subroutines for retrieving and loading pseudocomponent properties from the internal ASPEN storage for transfer from one process module to another are being developed. Integration of the subroutines into various FORTRAN block models has not yet been started.

The proposed Table of Contents for this task/topical report is shown in this report.
# ASPEN SIMULATION MODEL OF THE BASELINE DESIGN

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3.6 TASK VI

Task 6 concerns the development of a training manual and a training course for the process simulation model. The training course will include an overview of the system, modification of the reporting system, interfacing user models, modification of chemical properties, use of the cost and economics modules, specifying flowsheets, streams, components, properties, and convergence. Trainees will be instructed through the use of case study example problems.

- The ASPEN training course is scheduled for the week of March 23, 1992 at the DOE/PETC facilities in Pittsburgh.

- A first draft of the documentation of Task 6, the training manual, is being prepared. This will be used for the proposed DOE training session.
4. KEY PERSONNEL STAFFING REPORT

Key Personnel staffing report for this reporting period (December 23, 1991 through March 15, 1992) as required by DOE/PETC is included in Table 4-1 shown below.

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<th>Function</th>
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<td>S. N. Habash</td>
<td>Project Manager</td>
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</tr>
<tr>
<td>S. K. Poddar</td>
<td>Technical/Project Coordinator</td>
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<td>T. J. Reynolds</td>
<td>Project Secretary</td>
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<tr>
<td>J. J. Nicholas</td>
<td>Project Manager</td>
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<tr>
<td>S. J. Kramer</td>
<td>Principal Investigator</td>
<td>66</td>
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<tr>
<td>Arun Basu</td>
<td>Principal Investigator</td>
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</tr>
<tr>
<td>T. E. Myers</td>
<td>Principal Investigator</td>
<td>26</td>
</tr>
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* (Number of hours spent/total available working hours for December 23, 1991 through March 15, 1992) x 100.