U.S. Department of Energy
Federal Energy Technology Center

Refining and End Use Study of Coal Liquids

Contract No. DE-AC22-93PC91029

Quarterly Report
April - June 1997

Section 1

Introduction and Summary

Section 1

Introduction and Summary

This report is Bechtel's fifteenth quarterly technical progress report and covers the period of April 1, 1997 through June 30, 1997.

1.1 Introduction

Bechtel National Inc, with Southwest Research Institute, Amoco Oil R&D, and the M.W. Kellogg Co. as subcontractors, initiated a study on November 1, 1993, for the U.S. Department of Energy's (DOE's) Federal Energy Technology Center (PETC) to determine the most cost effective and suitable combination of existing petroleum refinery processes needed to make specification transportation fuels or blending stocks, from direct and indirect coal liquefaction product liquids. This 47-month study, with an approved budget of $4.4 million dollars, is being performed under DOE Contract Number DE-AC22-93PC91029.

A key objective is to determine the most desirable ways of integrating coal liquefaction liquids into existing petroleum refineries to produce transportation fuels meeting current and future, e.g. year 2000, Clean Air Act Amendment (CAAA) standards. An integral part of the above objectives is to test the fuels or blends produced and compare them with established ASTM fuels. The comparison will include engine tests to ascertain compliance of the fuels produced with CAAA and other applicable fuel quality and performance standards.

The final part of the project includes a detailed economic evaluation of the cost of processing the coal liquids to their optimum products. The cost analyses is for the incremental processing cost; in other words, the feed is priced at zero dollars. The study reflects costs for operations using state of the art refinery technology; no capital costs for building new refineries is considered. Some modifications to the existing refinery may be required. Economy of scale dictates the minimum amount of feedstock that should be processed.

To enhance management of the study, the work has been divided into two parts, the Basic Program and Option 1.

The objectives of the Basic Program are to:

- Characterize the coal liquids
- Develop an optimized refinery configuration for processing indirect and direct coal liquids
- Develop a LP refinery model with the Process Industry Modeling System (PIMS) software.

The work has been divided into six tasks.

Task 1 - Development of a detailed project management plan for the Basic Program
Task 2 - Characterization of four coal liquid feeds supplied by DOE
Task 3 - Optimization of refinery processing configurations by linear programming
Task 4 - Pilot plant analysis of critical refinery process units to determine yield, product quality and cost assumptions. Petroleum cuts, neat coal liquids, and coal liquids/petroleum blends will be processed through the following process units: reforming, naphtha and distillate hydrotreating, catalytic cracking and hydrocracking.

- Task 5 -Development of the project management plan for Option 1

- Task 6 - Project management of the Basic Program and Option 1

The objectives of Option 1 are to:

- Confirm the validity of the optimization work of the Basic Program
- Produce large quantities of liquid transportation fuel blending stocks
- Conduct engine emission tests
- Determine the value and the processing costs of the coal liquids

This will be done by processing the coal liquids as determined by the optimization work, blending and characterizing the product liquids, and running engine emission tests of the blends. Option 1 has been divided into three tasks.

- Task 1 -Based on the pilot plant and linear programming optimization work of the Basic Program, production runs of pilot plants (hydrotreating, reforming, catalytic cracking, and hydrocracking) will be conducted to produce sufficient quantities for blending and engine testing.
- Task 2 -The pilot plant products will be blended, characterized, and engine tested
- Task 3 -An economic analysis will be conducted to determine the costs of processing the coal liquids through the existing refinery

Table 1-1 shows which organization has the primary responsibility for each task.

1.2 Summary

The major efforts conducted during the second quarter of 1997 were in the areas of:

- Option 1 fuel blending
- Option 1 fuel testing

Table 1-1 Project Task Primary Responsibility Chart

Task	Description	Bechtel	SwRI	Amoco	Kellogg
1	Project Management Plan (PMP) development	x			
2	Feed characterization		x		
3	Linear programming	x			
4	Pilot plant analysis -				
	Cat cracking of DL liquids				x
	Cat cracking of indirect wax			x	
	Hydrocracking of wax			x	
	Fractionation, reforming, hydrotreating, etc.		x		
5	Option 1 PMP development	x			
6	Project management	x			
Option 1 - Task 1	Pilot plant production -				
	Cat cracking of DL liquids and wax				x
	All other production work		x		
Option 1 - Task 2	Fuel blending, characterizing, engine testing		x		
Option 1 - Task 3	Economic analysis	x			

- x = key participant

Section 2

SwRI Activities

2.0 Option 1 Test Fuel Production

The Option 1 test program required larger volumes of the test fuels than used in all of the previous Task 4 pilot plant tests. For example, the engine and combustor studies, with their associated emissions tests, use test fuel volumes in the tens of gallons range.

In earlier work, the actual properties of each available blendstock were provided to the PIMS (Process Industry Modeling System) linear programming model, along with the actual analysis of the reference fuel to be used in the performance tests, in order to determine a blend composition for each Option 1 test fuel. The iterative quality of this work is illustrated in Figure 2-1 in which the alternate flow of information from the physical work *to* PIMS and the return of targets, limits and parameters *from* PIMS served to guide the production. A detailed description of this work was provided in the "Option 1 Management Summary/Plan - Fuel Production/Engine Performance Testing", issued May 29, 1997.

The blend compositions provided by PIMS were used to produce the following slate of test fuels for engine and emissions testing:

- DL2 Highway Diesel
- DL1 Highway Diesel
- DL2 Off-road Diesel
- DL2 Jet A
- DL2 Conventional Regular Gasoline
- DL2 Reformulated Premium Gasoline

In the case of the diesel fuels, correct blending was verified by making a small trial batch before mixing the full volume of test fuel. These were designated "hand blends". Gasoline testing needed less volume of fuel, and each blend required more components, so the gasolines were carefully blended and tested at full scale. The gasoline properties agreed well with the projected properties, and no reblending was required.

Although blends were calculated in volumetric terms, the blend compositions were made by weight. Gravimetric measurements are easier to determine, can be read in greater accuracy, and reflect any losses immediately, for example, from evaporation. The final composition of each test fuel blend is given in Tables 2-1 through 2-6.

Though a prosaic part of the work, the assembly of the test fuels was done with great care. Over the course of the project, hundreds of sample ID numbers have been created, and the inventory of materials are located in cold boxes, indoor, and outdoor storage locations. Assuring the correct identity of each addition to the test fuel blends was of paramount importance. A further concern was the thorough mixing of the blends, which was assured by recirculation and mechanical agitation as needed.

2.1 Test Fuel Laboratory Evaluation

Before the test fuels were sent off for engine performance testing, the ASTM specification properties were measured. In addition to assuring that the formulations determined by PIMS were correctly implemented, the lab tests verified the operational properties that are part of the various ASTM specifications for each fuel type and grade. As discussed in earlier reports, the specifications used in this project were extrapolated to the near future, when environmental concerns for gaseous and particulate emissions may impose tighter limits on gasoline and diesel compositions. Thus key properties were made more restrictive than today’s values in the specifications. For instance, the highway diesel fuels were blended to conform to grade 2D of ASTM D 975-94, but with higher cetane index and lower sulfur content. The balance of the property specifications were assumed to at current levels for cleanliness, storage stability, and utilization variables, like pour point. The results of this testing are presented in Tables 2-7 through 2-12.

As can be observed from the comparisons in the tables, the experimental fuels did very well. This is in spite of the fact that the determination of the blend recipes only took key properties into consideration. The exception was the behavior of the Jet A in the thermal stability testing. For instance, the JFTOT rating of >4 is incompatible with the requirement of a rating of less than 3 in ASTM D 1655. In the JFTOT, the test fuel flows over a heated aluminium rod, which is then rated for its deposits on a scale of 1 to 4. The darker deposits come from higher molecular weight aromatics or even cycloparaffins. It was not determined how the petroleum-derived components influenced the JFTOT rating, so no inference may be made about the thermal stability of the DL2 components. The other properties are consistent with a good fuel.

The diesel fuels readily met specifications and demonstrate a set of successful diesel fuels containing direct liquefaction products. The gasolines also met specifications. Because of the oxygenate content, the heating values were less than would have been expected from the dense coal-derived components from which they were made. The lower heating value was not out of line with the oxygenate concentrations and was what would arise from petroleum-based blends with similar oxygenate concentrations. Standing in equal concern for eventual use of coal-derived fuels are acceptance issues including fuel odor. While the diesels were not distinctive, the gasolines and jet fuel possessed a trace of “coal tar” scent, which was noted by the technicians.

2.2 Test Fuel Performance Testing

Preparations were made for engine and combustor testing of the six, Option 1 test fuels. The performance tests will be rated by comparison with advanced petroleum test fuels obtained commercially. Therefore, reference fuel selections were ordered and are shown in Table 2-13 with the tests to be performed on each test fuel. The reference fuel selection was important for the program in two ways: 1) rigorously chosen test fuels give higher confidence to the evaluations of the coal-based test fuel and, 2) overqualified reference fuels would set an unreasonably high standard for the test fuels. By using commercial reference fuels, unaltered in this program, more credible results will be obtained and may present opportunities for more widespread recognition of the results of the tests. A check of the engine test cell schedule showed a testing slot was available for each type of performance test. The test fuels have been prepositioned at each appropriate test area so the work could commence at the earliest practicable moment. The results of this testing will be the subject of a future quarterly report.

Table 2-1. Formulation for DL2 Highway Diesel Fuel

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, Lb
Hydrotreated Petro Kerosene	FL-2605	12.92	0.8063	86.75
SR Petro Light Distillate	FL-2311	7.19	0.8196	49.10
SR DL2 Light Distillate	FL-2541	16.57	0.8638	119.20
Hydrotreated Petro Gas Oil + H. Dist.	FL-2636	67.52	0.8398	472.45
TOTAL	FL-2637	104.21	0.8381	727.3

Table 2-2. Formulation for DL1 Highway Diesel Fuel

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, Lb
Hydrotreated Petro Kerosene	FL-2605	5.84	0.8063	39.20
SR Petro Light Distillate	FL-2311	6.56	0.8196	44.80
SR DL1 Distillate	FL-2371	16.67	0.8762	121.65
Hydrotreated Petro Gas Oil + H. Dist.	FL-2636	75.13	0.8398	525.65
TOTAL	FL-2639	104.20	0.8591	731.10

Table 2-3. Formulation for DL2 Off-road Diesel Fuel

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, Lb
SR Petro Light Distillate	FL-2311	29.22	0.8192	199.35
SR DL2 Light Distillate	FL-2541	7.41	0.8638	53.30
Hydrotreated Petro Gas Oil + H. Dist.	FL-2636	32.53	0.8398	227.60
SR DL2 Heavy Distillate	FL-2539	16.16	0.9139	123.00
Cat Cracked DL2 Diesel	FL-2620	8.45	0.9785	68.85
Hydrocracker Diesel	FL-2349	10.43	0.8464	73.55
TOTAL	FL-2640	104.20	0.8591	745.55

Table 2-4. Formulation for DL2-Jet A

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, Lb
Hydrotreated Petro Kerosene	FL-2605	17.61	0.8063	118.25
SR Petro Light Distillate	FL-2311	5.474	0.8192	37.35
SR DL2 Light Distillate	FL-2541	8.893	0.8638	63.97
TOTAL	FL-2641	31.977	0.8245	219.57

Table 2-5. Formulation for Conventional Regular DL2 Gasoline

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, lb
DL2 Reformate	FL-2634	3.70	0.8121	25.02
Generic Isomerate	FL-2348	1.88	0.6763	10.60
Methyl tert Butyl Ether	MTBE	0.37	0.7405	2.276
Generic Alkylate	FL-2344	0.21	0.6972	1.202
FCC DL2 Depentanizer Bottoms	FL-2619	2.4	0.7910	15.82
Refinery Butanes (Obtain RVP = 8.0-8.7)	Butane	0.45	0.58	~2.18
TOTAL	FL-2642	~9	-	57.10

Table 2-6. Formulation for Reformulated Premium DL2 Gasoline

Component	ID Number	Volume, Gal	Sp. Gr.	Weight, lb
Generic Alkylate	FL-2344	5.23	0.6972	30.36
DL2 Reformate	FL-2634	0.37	0.8121	2.50
Generic Isomerate	FL-2348	0.10	0.6763	0.558
Methyl tert Butyl Ether	MTBE	1.02	0.7405	6.28
Pet Hydrocracker Light Naphtha	FL-2351	0.21	0.7675	1.323
FCC DL2 Depentanizer Bottoms	FL-2619	2.09	0.7910	13.76
Refinery Butanes (Obtain RVP = 8.0-8.7)	Butane	0.21	0.58	~1
TOTAL	FL-2643	~9		55.78

Table 2-7. Analytical Evaluation of DL2 Highway Diesel Fuel

Property	Test Method	Property Specification ASTM D 975mod Min / max	Results	
ID Number			LN 858	FL2637
Designation			Hand Blend	Full Blend
Sp. Gravity	D 4052	>0.8324/<0.8488	0.8386	0.8385
API Gravity		>35.2/<38.5	37.2	37.3
Density, G/mL		>0.8317/<0.8401	0.8381	0.8380
Sulfur, M%	D 2622	<0.0412	0.044	0.043
Hydrocarbon Type	D 1319			
Aromatics, V%				22.1
Olefins, V%				1.2
Saturates, V%				76.7
Cetane No.	D 613		44.5	42.8
Cetane Index	D 976/D 4737	>46.3	46.6	47.8/47.5
Pour Point, F	D 97	<-5	-15	-9
Viscosity, 40 C	D 445	>1.9/<4.1		2.22
Distillation	D 86			
IBP/10%			338/402	336/400
30%/50%			445/480	446/487
70%/90%		- / 540 - 640	519/567	528/580
EP			593	626

SwRI Activities

Table 2-8. Analytical Evaluation of DL1 Highway Diesel Fuel

Property	Test Method	Property specification ASTM D 975mod Min / max	Results	
ID Number			LN 857	FL2639
Designation			Hand Blend	Full Blend
Sp. Gravity	D 4052	>0.8324/<0.8488	0.8428	0.8429
API Gravity		>35.2/<38.5	36.4	36.3
Density, G/mL		>0.8317/<0.8401	0.8423	0.8424
Sulfur, M%	D 2622	<0.0412	0.043	0.041
Hydrocarbon Type	D 1319			
Aromatics, V%				25.2
Olefins, V%				1.8
Saturates, V%				73.0
Cetane No.	D 613		45.1	42.5
Cetane Index	D 976/ D4737	>46.3	46.8	47.6/47.4
Pour Point, F	D 97	< -5	-10	-5
Viscosity, 40 C	D 445	>1.9/<4.1		2.33
Distillation	D 86			
IBP/10%			345/417	394/412
30%/50%			458/491	459/498
70%/90%		- / 540 - 640	527/574	534/582
EP			611	629

Table 2-9. Analytical Evaluation of DL2 Off-Road Diesel Fuel

Property	Test Method	Property Specification ASTM D 975mod Min / max	Results	
ID Number			LN 859	FL2640
Description			Hand Blend	Full Blend
Sp. Gravity	D 4052	<0.8612	0.8598	0.8578
API Gravity		>32.8	33.1	33.5
Density, G/mL		<0.8605	0.8593	0.8573
Sulfur, M%	D 2622	<0.24	0.247	0.269
Hydrocarbon Type	D 1319			
Aromatics, V%				30.3
Olefins, V%				0.9
Saturates, V%				68.8
Cetane No.	D 613		40.5	41.1
Cetane Index	D 976/ D 4737	>41.4	42.0	42.4/41.7
Pour Point, F	D 97		-17	-7
Viscosity, 40 C	D 445	- / 540 - 640		2.26
Distillation	D 86			
IBP/10%			343/413	343/411
30%/50%			459/495	455/493
70%/90%			538/593	533/589
EP			641	649

Table 2-10. Analytical Evaluation of Jet A Test Fuel

Property	Test Method	Property specification ASTM D 1655 Min / max	Results	
ID Number			LN 860	FL2641
Designation			Hand Blend	Full Blend
Sp. Gravity	D 4052	>0.7927/<0.8397	0.8264	0.8253
API Gravity		>37.0/<47.0	39.7	40.0
Density, G/mL		>0.7920/<0.8390	0.8260	0.8249
Sulfur, M%	D 2622	<0.1	0.0840	0.107
Hydrocarbon Type	D 1319			
Aromatics, V%		<19.5	17.4	17.8
Olefins, V%			1.8	0.7
Saturates, V%			80.8	81.5
Smoke Point, mM	D1322	>19.0*	22.0	20.2
Naphthalenes	D1840	<3.0		0.72
Freezing Point, F	D2386	<-40	-62	-60
Viscosity, 40 C	D 445			1.51
Distillation	D 86			
IBP/10%		- /<401	337/376	332/372
30%/50%			402/422	398/422
70%/90%			448/488	444/488
EP		<572	528	533

* Smoke Point specification > 19.0 required if naphthalenes are less than 3.0 %

Table 2-11. Analytical Evaluation of DL2 Gasolines

Property	Property specification Reg / prem	Results	
Designation		Conventional Regular	Reformulated Premium
Sp. Gravity	0.7479 - 0.7503	0.7583	0.7249
Api Gravity	57.7 - 57.1	55.1	63.7
Density, G/ml	0.7472 - 0.7496		
Sulfur, m%	<0.0339	0.0386	0.0392
Hydrocarbon Type			
Benzene, v%	<1.0	1.01	0.51
Aromatics, v%		32.4	15.4
Olefins, v%		1.0	1.2
Saturates, v%		66.6	83.4
Rvp, Psi	<8.7	8.63	8.62
Octane No. Ron		91.2	94.0
Mon		83.9	87.9
(R+M)/2	87 / 92	87.5	91.0
Distillation			
IBP/10%		92/130	91/133
30%/50%	- / >~211	182/235	176/211
70%/90%	- / >~319	281/332	243/325
EP		392	399

Table 2-12. Additional Properties of Option 1 Test Fuels

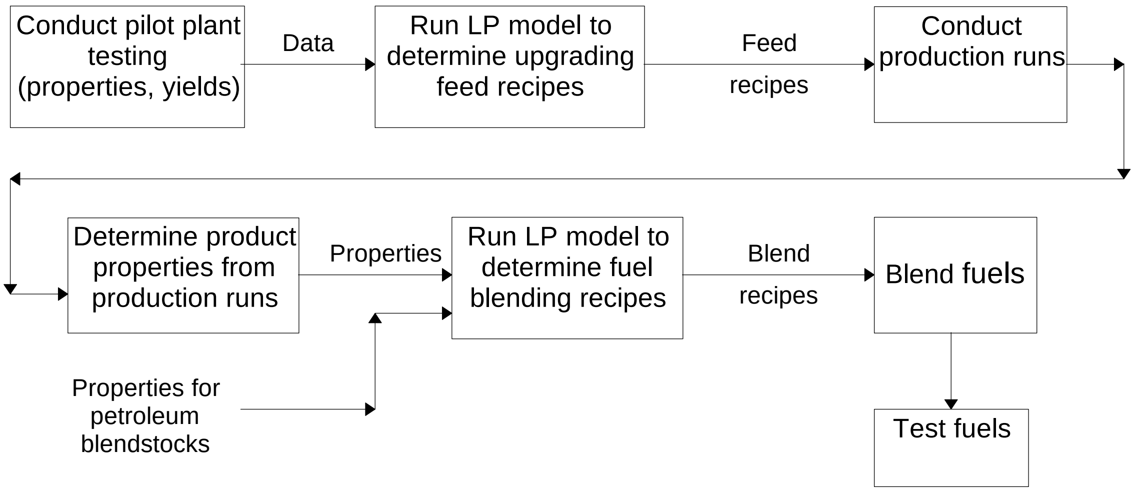
Fuel Description	Diesel				Gasoline	
	Highway	Highway	Off road	Jet A	Conv. Reg	Reform. Prem
Source	DL1	DL2	DL2	DL2	DL2	DL2
Test Description						
Sulfur, ppm	430	410	2690	1070	386	392
Existent Gum, mG/100mL unwashed				2.9	2.5	1.5
washed				2.6	2.1	1.0
Flash Point, F	140	144	146	124		
Cloud Point, F	-6	-8	-10			
Freezing Point, F				<-40		
Carbon Residue, Wt%	0.05	0.06	0.09			
Net Heating Value, BTU/lb				18498	18447	18489
Oxidation Stability, min					>1440	>1440
Ash, Wt%	<0.001	<0.001	<0.001			
Total Acid Number				<0.01		
Thermal Stability, visual				>4		
8A Spun rating				37		
8A Spot rating				39		
Hydrogen, Wt%	13.47	13.33	12.92	13.63	12.98	14.82

Table 2-13. Option 1 Combustion and Emission Testing Sequences

Type		Reference Fuel	Tests
Diesel	DL1, Highway	Phillips 2, W-240	EMA/EPA Protocol Calc FTP NOx CVCA ASTM
	DL2, Highway	Phillips 2, W-240	
	DL2, Off-road	Phillips CN40	
Jet	DL2, Jet A	Commercial Jet A	T-63 Combustion ASTM
Gasoline	DL2, Conventional Regular	Phillips 1990 Baseline Reference	FTP Transient Cycle ASTM
	DL2, Reformulated Premium		

SwRI Activities

Figure 2-1 - Work Sequence to Produce the Option 1 Blend Formulations



Section 3

Bechtel Activities

There was no project activity for this reporting period.

Section 4
Amoco Activities

There was no project activity for this reporting period.

Section 5

M.W. Kellogg Activities

There was no project activity for this reporting period.

Section 6

Project Management

6.1 Reports and Schedules

The milestone schedule and status for the Basic Program and Option 1 is shown in Figure 6-1.

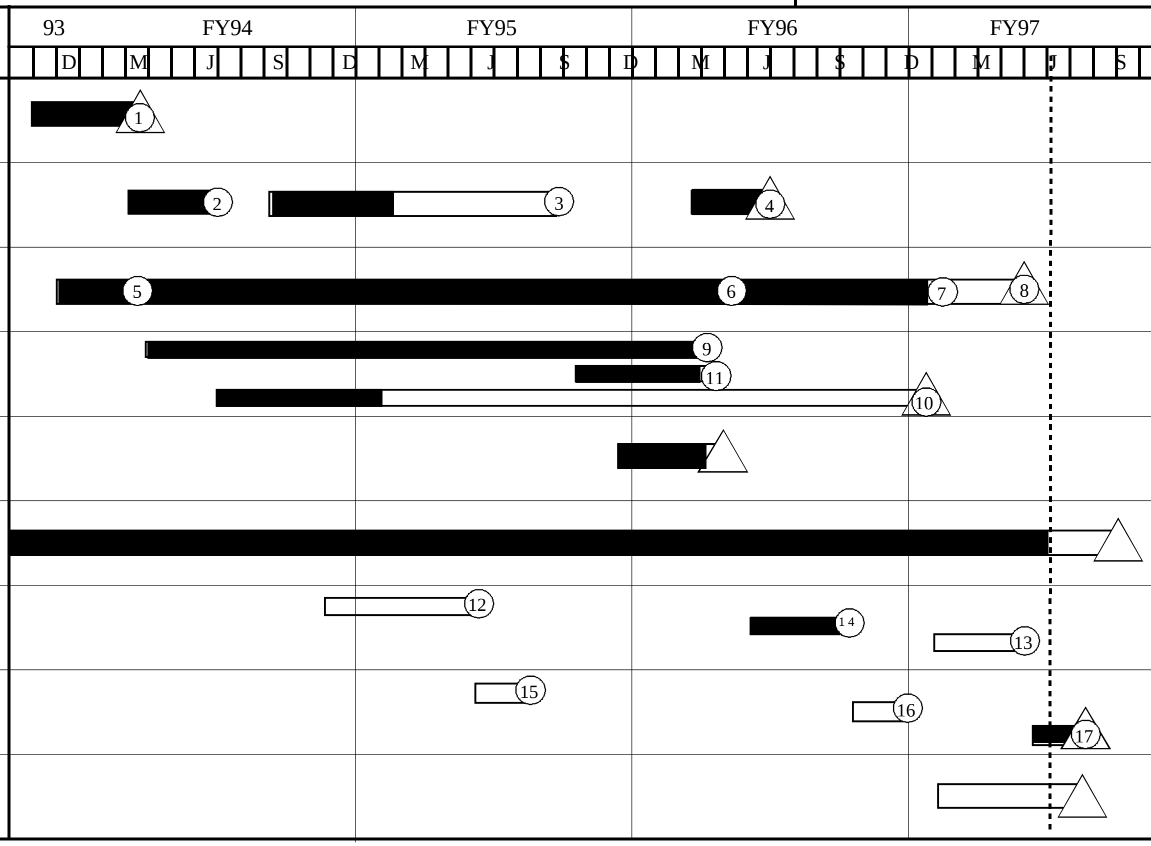
DOE F1332.3
(11.84)

FORM APPROVED
OMB NO 1901.1400

Figure 6-1
Milestone Schedule for Basic Program & Option 1

☐ PLAN ■ STATUS REPORT

1. TITLI Refining and End Use Study of Coal Liquids	2. REPORTING PERIOD 4/1/97 to 6/30/97	3. IDENTIFICATION NUMBER DE-AC22-93PC91029
4. PARTICIPANT NAME AND ADDRESS Bechtel Corporation, 50 Beale Street, San Francisco, CA 94105		5. START DATE 11/1/93
		6. ESTIMATED COMPLETION DATE 9/30/97



7. ELEMENT CODE	8. REPORTING ELEMENT	10. PERCENT COMPLETE a. Plan	b. Actual
Task 1	Project Work Plan	100	100
Task 2	Feed Characterization	100	70
Task 3	Linear Programming (LP) Analysis	100	82
Task 4	Pilot Plant Analysis	100	75
Task 5	Option 1 Work Plan	100	80
Task 6	Administration Task	85	85
Option 1 Task 1	Pilot Plant Analysis (Produce Fuels)	100	33
Option 1 Task 2	Characterization, Blending, and Testing	10	100
Option 1 Task 3	Economic Study	30	20

1 Submit Final Work Plan
2 Characterize DL1 liquid
3 Characterize IL liquid
4 Characterize DL2 liquid
5 Develop LP model
6 Input DL pilot plant data
7 Input IL pilot plant data
8 Conduct evaluation runs
9 Conduct DL1 pilot plant tests
10 Conduct IL pilot plant tests
11 Conduct DL2 pilot plant tests
12 Production runs for DL1 (deleted from program)
13 Production runs for IL(deleted from program)
14 Production runs for DL2
15 ASTM tests for DL1 (deleted from program)
16 ASTM tests for IL(deleted from program)
17 ASTM tests for DL2

11. SIGNATURE OF PARTICIPANT'S PROJECT MANAGER AND DATE