**Exploratory Research on Novel Coal
Liquefaction Concept**

**Quarterly Technical Progress Report
July 1 through September 30, 1998**

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CONTRACTOR NAME:

CONSOL Inc.
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4000 Brownsville Road
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PRINCIPAL INVESTIGATORS: R. A. Winschel, S. D. Brandes

SUBCONTRACTORS/PRINCIPAL INVESTIGATORS:

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CONTRACTING OFFICER'S REPRESENTATIVE: M. A. Nowak

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CONTRACT OBJECTIVES: No Change

SUMMARY OF TECHNICAL PROGRESS - OVERALL

All experimental testing for the contract was completed. Economic evaluations for the conceptual process are under way.

SUMMARY OF TECHNICAL PROGRESS BY TASK

Task 4 - Integrated Flow Sheet Testing

First-Stage Tests

All first-stage tests are complete.

Second-Stage Catalytic Upgrading

Second-stage catalytic upgrading experimentation is complete. Duplicate samples of 41-LA series feeds and products were analyzed and the results were forwarded to LDP.

Filtration

It was reported last quarter that filtration rates between 10 kgm²/h and 33 kgm²/h were achieved with post-second-stage filtration. It was estimated that a filtration rate of 30 kgm²/h would give a base cost of ~\$1.6 bbl oil compared with \$0.48 bbl oil calculated for interstage filtration rates of 100 kgm²/h. The base cost of post-upgrading filtration could be reduced by pre-distilling the unfiltered hydrotreater product to increase the solids loading to the filter from 6% to 12%. This would reduce the amount of filtrate per unit of coal feed by a factor of 2.25, with a reduction in base cost for filtration to \$0.70 bbl oil. To compensate for the increase in viscosity, a higher filtration temperature would be used; this is possible because the second-stage products do not have a low-boiling volatile component, as does the interstage material.

A sample of the combined Run 41bcLA first-stage product, was combined with a commercially available carbonaceous filter aid to examine the effect on the filtration rate. The filter aid was used at a loading of 2.5%. Rates obtained with Run 30-LA products, which were prepared under identical conditions as 41bcLA, were used for comparison. Run 30-LA products gave a filtration rate of 62 kgm²/h. A filtration rate of just over 100 kgm²/h was achieved, almost double the rate observed with the Run 30-LA product.

These tests completed all experimental work for the contract.

Task 5 - Engineering and Economic Study

The first-stage Run 41 series elementally balanced material balances and net yields by boiling range were revised to reflect the SO₃-free ash content of the feeds and products and the topping of the first-stage product prior to SIMDIST analysis. The revised results are shown in Table 1.

Elementally balanced material balances and net yields by boiling range were prepared for the second-stage tests made with the first-stage Run 41 series products. The balances and yields reflected the SO₃-free ash content of the feeds and products. In preparing the balances, it was necessary to develop a method for correcting the as-measured yield and elemental analysis of the scrubber distillate to account for its much higher-than-expected sulfur, nitrogen, and oxygen concentrations. The method estimated the quantities of unreacted DMDS and dissolved

heteroatom compounds (i.e., H_2S , NH_3 , and H_2O) contained in scrubber distillate so that they could be subtracted from the as-measured values.

A second correction to the above balances and yields is required to account for the much lower-than-expected net methane yield (methane out, less methane formed from DMDS decomposition). The net methane yield was negative in two of the four runs and lower than expected in the two other runs. However, the yields of ethane plus propane per unit of resid converted were approximately constant. Data from pilot-scale coal liquefaction units indicates that the expected methane yield is approximately 75% of the combined ethane plus propane yield per unit of resid converted. The methane yield was adjusted on this basis.

Elementally balanced material balances and net yields by boiling range for Run 263J-2, 300 CSTR, were prepared based on the experimental data. Resid conversion data from this run were compared to those obtained in the Novel Concept run at the same reaction conditions to determine the relative reactivity of the Novel Concept resid vs. the Base Case (Wilsonville Run 263J) resid.

Work on the evaluation of the Novel Concept Conceptual Commercial Plant Case (T4NCC) based on the Task 4 experimental results (Run 41 series) was begun. The following were completed:

- Integrated liquefaction system material balance
- Liquefaction distillate upgrading balance
- First-stage CO make-up, recover, and recycle system balance
- Second-stage hydrogen make-up, recovery, and recycle system balance
- Gasification system heat and material balances
- First- and second-stage reactor systems heat balances and reactor sizing
- Fuel balance and C_4 LPG by-product rate
- Electrical power requirements and internal power production rate
- Estimated capital costs for nine of the fifteen process units.

Task 6 - Reporting

A quarterly review meeting was held with project participants at CONSOL R&D in Library, PA, on July 8. A review meeting with DOE (M. Nowak, Contract COR) was held on July 15, 1998. Meeting reports were issued. The Task 4 Topical Report/Final Report is being drafted. A journal paper was drafted describing Task 2 first-stage coal dissolution test results. Reporting is on schedule.

FORECAST AND PLANS

All Task 4 experimental testing is complete. The economic evaluation of the Novel Concept Conceptual Commercial Plant based on Task 4 results will be completed. A draft of the Task 4/Final Report will be completed and sent to DOE for approval. Additional journal papers are planned; these will describe the filtration work and the overall process design for the Novel Concept process.

TABLE 1

RUN 41 SERIES FIRST-STAGE NET YIELD SUMMARY

Net Yields: wt % MF Coal

	Run 41o	Run 41a	Run 41b	Run 41c	Run 41 Avg	Run 23dfg Avg
H ₂ O	-11.26	-10.31	-8.87	-9.66	-10.03	-23.64
NH ₃	0.00	0.01	0.35	0.25	0.15	0.03
H ₂ S	0.00	0.32	0.00	0.04	0.09	0.09
H ₂	1.12	0.55	0.63	0.45	0.69	2.30
CO	-17.66	-16.18	-13.94	-15.17	-15.74	-37.16
CO ₂	40.35	37.27	34.84	33.30	36.44	74.20
C ₁ -C ₃	0.62	0.47	0.54	0.51	0.54	0.58
C ₄ -C ₅	0.08	0.05	0.04	0.05	0.06	0.03
IBP-150 °C	0.42	0.44	0.52	0.45	0.46	0.35
150-200 °C	-0.14	-0.33	0.78	0.64	0.24	-0.35
200-250 °C	-0.33	-1.04	1.32	0.94	0.22	-3.70
250-300 °C	0.92	0.71	0.22	0.10	0.49	-0.20
300-350 °C	2.90	2.70	2.51	3.13	2.81	6.78
350-400 °C	3.10	3.41	3.45	4.63	3.65	7.09
400-450 °C	2.07	2.38	0.60	1.32	1.59	3.47
450-500 °C	2.66	2.78	2.57	2.93	2.74	3.63
500-566 °C	3.32	3.47	4.77	4.86	4.11	4.77
THFS 566 °C ⁺	30.30	30.97	29.96	30.69	30.48	42.69
THF IOM	36.13	36.93	34.31	35.14	35.63	13.74
SO ₃ -Free Ash	6.02	6.02	6.03	6.02	6.02	6.55
Total	100.62	100.62	100.63	100.62	100.62	101.25
<u>% Coal Conversion</u>						
THFI Basis	61.8	60.9	63.7	62.8	62.3	85.5
QI Basis	83.1	82.7	86.7	86.4	84.7	91.9
% Coal Deoxygenation	50.3	47.3	51.6	37.8	46.8	60.0
C ₄ -300 °C	0.96	-0.18	2.88	2.17	1.46	-3.87
C ₄ -566 °C	15.00	14.56	16.78	19.04	16.35	21.87
AF 566 °C ⁺	66.43	67.90	64.27	65.83	66.11	56.43

7/31/98 Revised for topping of Rec/Auto and SO₃-free ash basis