

A test of product slate flexibility is tentatively planned for the next run. This would eliminate the higher boiling point fraction of the system product by extinction recycle with the recycle process solvent.

The coal liquefaction database is being enhanced by continuing efforts in process modeling and simulation.

The feasibility of using the Wilsonville facility for study of coprocessing has been investigated. The facility appears to be ideally suited for operation as a coprocessing unit.

#### RELATIVE ECONOMIC EVALUATION

An important extension of the process evaluation is to apply what has been learned about process performance to the process economics.

The economic data developed by Lummus Crest Inc. (LCI) under a contract from the Electric Power Research Institute (EPRI) and Hydrocarbon Research, Inc. (HRI) under a contract from the Department of Energy (DOE) is used to make relative economic comparisons among several processes. In the Lummus study a method was developed to evaluate and compare processes on a consistent basis (8).

The economic evaluations were based on actual dollar estimates for capital cost, operating costs and production costs. Since these costs are based on many assumptions the actual costs are not so important in the absolute sense. However the relative economics are a good indicator of how the processes compare to one another.

One conclusion that can be made is that all the processes are capital intensive. The high required selling price of synthetic fuels and the current projected price of crude oil make these processes non-competitive in the current economic situation. However, the information presented will show that significant improvements are being made in process development.

The processes presented will be compared to the H-Coal process (Slide 20) as a baseline. The H-Coal process utilizes a single ebullated bed catalytic reactor to accomplish 1) coal conversion to resid, 2) resid conversion to distillate products

and 3) product quality. The solids are removed from the system via the vacuum column bottoms which is fed to a gasifier to produce the hydrogen gas used in the process. The net products are gasoline and a low sulfur No. 6 fuel oil.

The next advance in the process development was a two stage system employing a thermal reactor for coal conversion to resid and an ebullated bed catalytic reactor to hydrogenate the solvent and convert the resid to distillate products. The advantage of this concept is that the reaction severity of each stage can be independently controlled to obtain the desired level of coal conversion and the desired level of resid conversion somewhat independent of one another.

The first step in the two-stage liquefaction development was the non-integrated two stage liquefaction (NTSL) mode (Slide 21). In this mode the recycle streams are contained within each stage. The major product from the NTSL operation is a synthetic fuel oil which is a blend of 60 percent distillate and 40 percent resid shown to be equivalent to No. 6 fuel oil (2).

As the interest in more distillate products increased, the ITSL mode of integration was employed in which the resid was recycled to extinction (Slide 22). In this mode the first and second stages are integrated in that the resid and part of the solvent from the second stage are recycled to the first stage reactor. This mode of operation provides an all distillate product slate, good hydrogen utilization efficiency and reasonable organic rejection with the ash removal stream, and some improvement in product quality.

A reconfigured integrated two stage liquefaction (RITSL) mode (Slide 23) was the next step in the process development. In this mode first stage vacuum tower bottoms containing ash, resid and solvent are fed directly to the second stage. The deashing step is carried out after hydrotreating. This configuration was an intermediate step leading to the direct coupling of the first and second stage reactors. The benefits of the RITSL operation were data showing no adverse affect on the second stage catalyst, improved product quality and a reduction in the size of the deashing unit due to the conversion of more of the resid in the second stage prior to the deashing step.

The RITSL configuration led directly to the close-coupled integrated two stage liquefaction (CC-ITSL) shown in Slide 24. The major change between RITSL and CC-ITSL is the elimination of the interstage pressure letdown and solvent recovery systems

and the subsequent repressuring and reheating of the feed to the second stage reactor. The two stages are directly coupled with only a vent separator between the reactors. The benefit derived from this configuration is improved energy efficiency leading to a reduction in operating costs associated with the process.

The relative economics among these processes are shown in Slide 25. The total plant/construction cost and the total capital required increases as the plants become more sophisticated in their modes of integration.

There are many cost trade-offs and differences among the processes. In comparing H-Coal to NTSL there is only a 16 percent increase in the NTSL reaction section cost even though the NTSL system is a two stage system and H-Coal is a single stage system. The deashing costs are much higher in NTSL. This capital cost is more than offset by decreases in capital for gasification and electrical power generation for the H-Coal plant.

Comparing ITSL to NTSL a major increase in capital is required. The major cost increase occurs in the reaction sections, up 42 percent, with smaller increases in deashing, off gas clean up and compression and gasification. The addition of resid recycle requires additional plant capacity throughout the plant. Increased hydrogen consumption required for resid extinction increases costs for gasification which is the source of hydrogen for the process.

The subsequent increase of cost in the CC-ITSL mode results from the increased feed to the second stage in this mode and an increase in the hydrogen consumption. Both the reaction section and the gasification costs increase. A small decrease in deashing cost is realized since more of the resid is converted to distillate therefore less material is fed to the deashing unit.

Operating costs which varied the most between the various processes are coal cost, purchased electrical power, catalyst replacement costs and deashing solvent costs. (Note: All cases utilized the Kerr-McGee critical solvent deashing (CSD) system for ash removal except the H-Coal case.)

The major differences between H-Coal and NTSL are the increases in the cost of purchased electrical power and deashing solvent.

The major operating cost increase when comparing ITSL to NTSL are: 1) increased coal cost because coal is required as feed to the gasifier as hydrogen consumption increases; 2) higher replacement catalyst cost when recycling resid to extinction; 3) additional deashing solvent cost due to resid recycle and 4) additional purchased electrical power requirements.

The annual production costs are a direct extrapolation of capital related costs plus operating cost and the method used to finance the plant and liquidate the debt. The ratios presented are based on first year requirements.

The annual production rate is based on barrels of crude oil equivalent (COE). The COE value is determined by taking into account the production rate of a given product and the product quality. Product quality is based on hydrogen and heteroatom content. For example, if a process yielded 10,000 barrels of naphtha a year and the calculated value relative to crude oil was 1.16 based on hydrogen and heteroatom content then the resultant yield for comparison purposes would be 11,600 barrels of crude oil equivalent. Conversely if a product has a relative value less than crude oil its yield would be decreased proportionately. As process integration progressed toward CC-ITSL the yields increased both in actual production of distillate products and in the quality of the distillates. This results in significant yield increases in terms of the COE.

The first year product required selling price is directly reflected in this increase yield of distillates and quality of the distillate. When yield and quality of the distillate is maintained and capital and operating costs do not change significantly an improvement is realized relative to the initial selling price required.

The relative cost factors as shown in Slide 25 have been developed using the most conservative design from the available sources and are based on the yield and throughput data from Run 247 at Wilsonville. Design conservatism generally translates to higher cost requirements. Another equally probable case has been developed from the available data which indicates that the advancements in the coal liquefaction technology have resulted in a 14% decrease in required selling price over the H-Coal case through Run 247 (Slide 26).

Further process configurations are currently being evaluated. As indicated, Run 250 has just been completed at Wilsonville in which cresol insolubles, ash and unconverted coal, were recycled in the process (Slide 27). This method of operation

allows the cresol insoluble material to be concentrated at a higher level in the CSD unit feed. Less total material is fed to the CSD unit and the required size of the CSD is significantly reduced. During the screening run, the feed to the CSD unit was reduced by 50%. An added benefit of that operation was improved TSL resid recovery which led to increased distillate yield. Organic rejections as low as 15% were observed. Another possible result of ash recycle is the elimination of the CSD unit entirely as demonstrated with subbituminous coal and ash removal is made by a vacuum tower bottoms. The factors affecting the feasibility of this possibility are ultimate levels of solids concentration that can be pumped in the vacuum bottoms system. This is dependent not only on solids loading but liquid viscosities.

Relative cost factors have been developed from the available data base reflecting these recent developments as demonstrated in Run 250 (Slide 28). This indicates that the advances in coal liquefaction technology have led to a reduction in required selling price of the products of approximately 20%.

#### CONCLUSIONS

Significant progress has been made in coal liquefaction process development with positive results as related to improved economics. Continued development work with catalyst and plant configurations should be continued. A detailed capital cost study needs to be undertaken to be able to better evaluate the many trade-offs that must be considered within the selected processes to be considered.

## REFERENCES

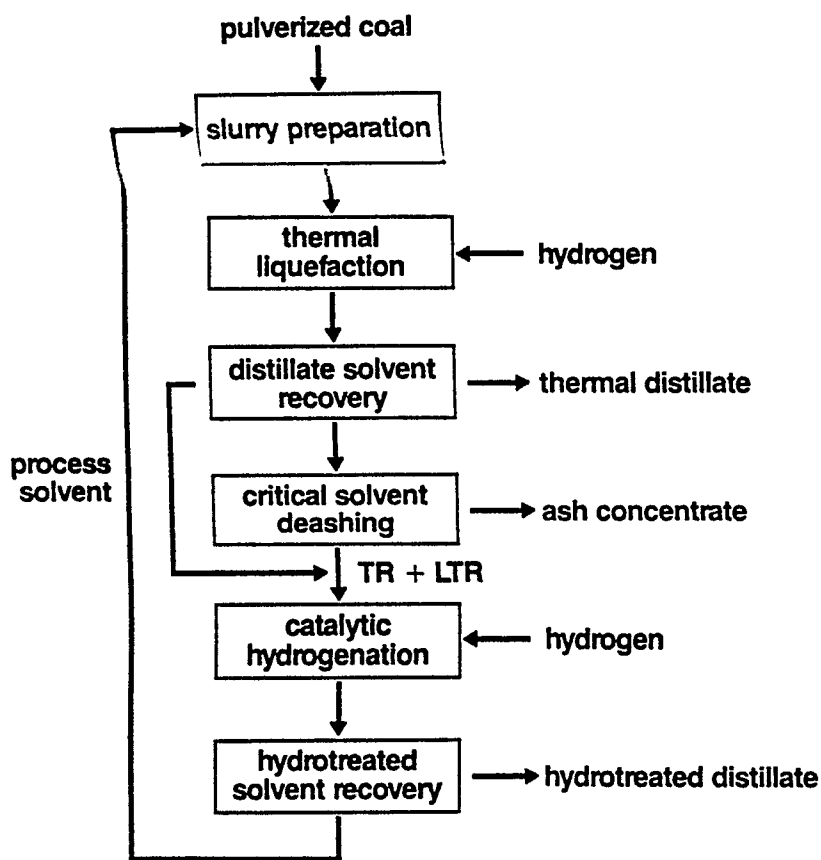
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## two-stage liquefaction integrated mode (ITSL)

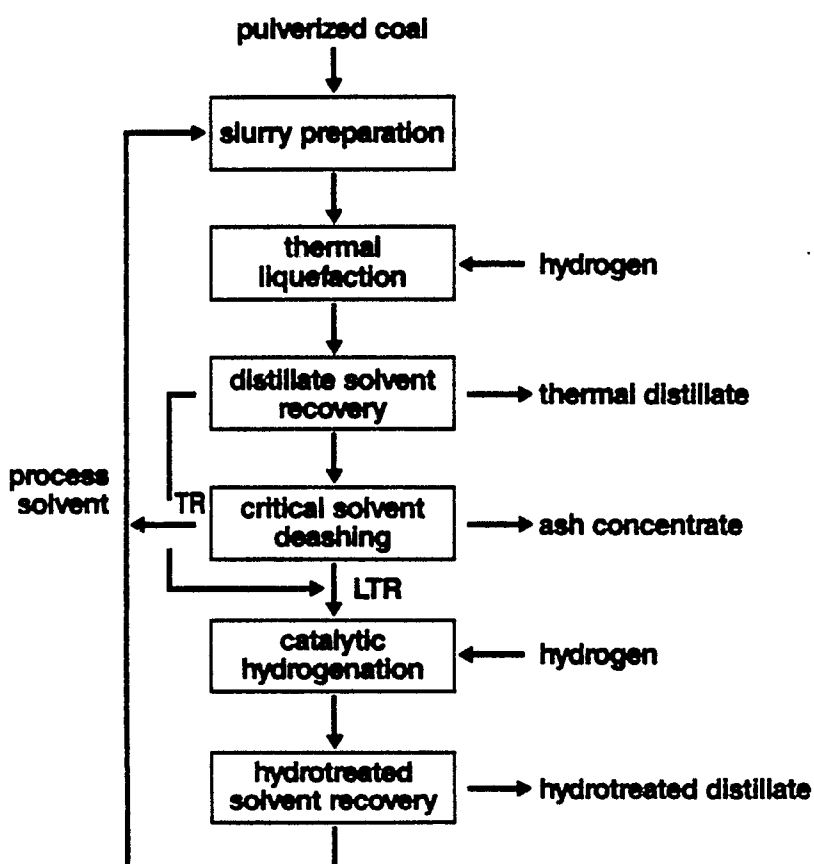


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## two-stage liquefaction double-integrated mode (DITSL)



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**run 248**

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**features**

- Illinois no. 6 coal
- LCT dissolver
- DITSL and ITSL configurations
- catalysts  
dissolver - iron oxide  
hydrotreater - unimodal NiMo

**results**

- DITSL operation difficult
- ITSL operation satisfactory
  - high distillate yield
  - increasing coal space velocity
  - lowered coal conversion
  - lowered distillate yield
  - yield similar to SCT

**low contact time (LCT) studies  
DITSL vs ITSL comparison**

**TSL operating conditions**

run no.	248A	248D
configuration	DITSL	ITSL
<b>thermal stage*</b>		
average reactor temperature (°F)	832	834
inlet hydrogen partial pressure (psi)	2040	2040
coal space velocity [lb/hr-ft <sup>3</sup> (>700°F)]	32	31
solvent-to-coal ratio	1.8	1.8
solvent resid content (wt %)	45-51	45
<b>catalytic stage</b>		
reactor temperature (°F)	648	705
space velocity (lb feed/hr-lb cat)	0.6	0.7
feed resid content (wt %)	39	57
catalyst age [(lb resid)/lb cat]	37-70	260-287

\*addition of Fe<sub>2</sub>O<sub>3</sub> at 2.0% MF coal and DMDS at 1.1 × stoichiometric requirement for conversion of Fe<sub>2</sub>O<sub>3</sub> to FeS

**low contact time (LCT) studies  
DITSL vs ITSL comparison**

**TSL yield structures**

run no.	248A	248D
configuration	DITSL	ITSL
<b>yield* (% MAF coal)</b>		
C <sub>1</sub> -C <sub>3</sub> gas (total gas)	7(13)	8(13)
water	8	8
C <sub>4</sub> + distillate	45	64
resid	18	3
hydrogen consumption	-4.7	-5.6
<b>hydrogen efficiency (lb C<sub>4</sub>+ dist/lb H<sub>2</sub> consumed)</b>	9.7	11.3
<b>distillate selectivity (lb C<sub>1</sub>-C<sub>3</sub>/lb C<sub>4</sub>+ dist)</b>	0.15	0.12
<b>energy content of feed coal rejected to ash conc. (%)</b>	24	19

\*elementally balanced yield structures



**LCT vs SCT comparison****TSL operating conditions**

	248F	242BC
run no.	248F	242BC
configuration	ITSL	ITSL
TLU reactor	LCT	SCT

**thermal stage**

average reactor temperature (°F)	835	860*
inlet hydrogen partial pressure (psi)	2040	2040
coal space velocity [lb/hr-ft <sup>3</sup> (>700°F)]	44	43

**catalytic stage**

reactor temperature (°F)	728	720
space velocity (lb feed/hr-lb cat)	0.7	1.0
catalyst age [(lb resid)/lb cat]	359-396	278-441

\*preheater outlet temperature

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**LCT vs SCT comparison****TSL yield structures**

	248F	242BC
run no.	ITSL	ITSL
configuration	LCT	SCT
TLU reactor		
<b>yield* (% MAF coal)</b>		
C <sub>1</sub> -C <sub>3</sub> gas (total gas)	7(12)	4(9)
water	9	10
C <sub>4</sub> + distillate	54	54
resid	8	8
hydrogen consumption	-5.3	-4.9
<b>hydrogen efficiency (lb C<sub>4</sub>+ dist/lb H<sub>2</sub> consumed)</b>	10.2	11.0
<b>distillate selectivity (lb C<sub>1</sub>-C<sub>3</sub>/lb C<sub>4</sub>+ dist)</b>	0.12	0.07
<b>energy content of feed coal rejected to ash conc. (%)</b>	23	23-27

\*elementally balanced yield structures

**run 249**

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**features**

- Wyodak coal
- dissolver back-mixed
- RITSL configuration
- catalysts  
dissolver - iron oxide and water  
hydrotreater - unimodal NiMo

**results**

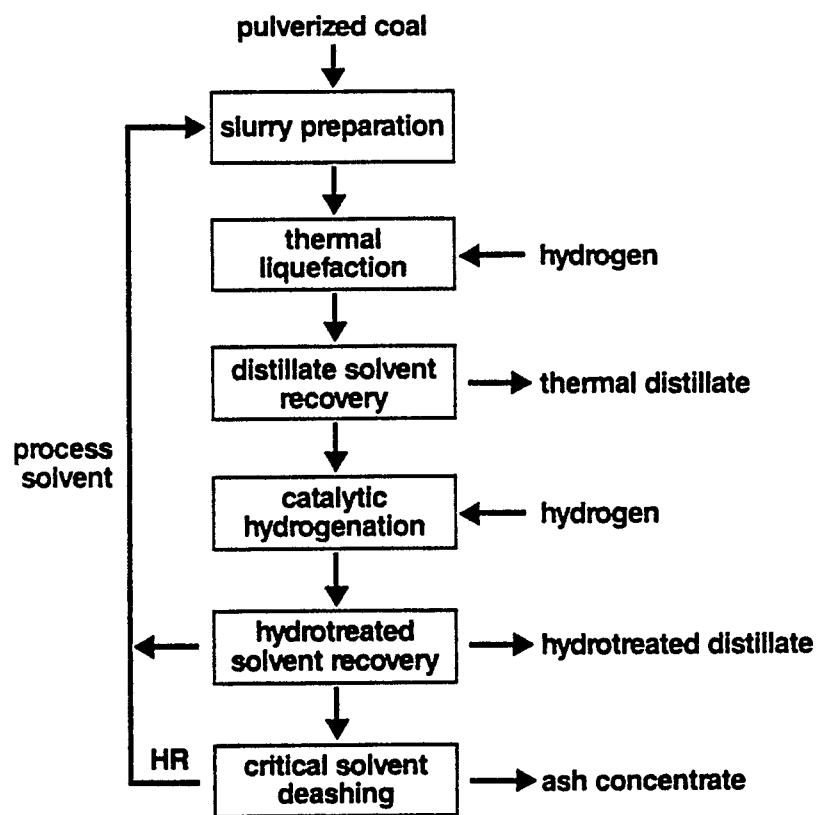
- iron oxide increased coal conversion
- water addition  
small conversion increase  
changed CSD feed  
similar overall yields
- ash recycle eliminated deashing step

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## two-stage liquefaction reconfigured mode (RITSL)



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## RITSL operating conditions (water addition & ash recycle)

run no.	249D	249E	249H*
<b>thermal stage</b>			
average reactor temperature (°F)	796	796	802
inlet hydrogen partial pressure (psi)	2040	2040	2040
coal space velocity [lb/hr-ft <sup>3</sup> (>700°F)]	14	14	14
solvent-to-coal ratio	1.5	1.5	2.0
solvent resid content (wt %)	30	29	22
iron-oxide addition**	yes	yes	yes
DMS addition	no	no	no
water addition	yes	no	no
<b>catalytic stage</b>			
reactor temperature (°F)	700	700	700
space velocity (lb feed/hr-lb cat)	1.3	1.2	1.6
feed resid content (wt %)	35	34	27
catalyst age [(lb resid + UC + ash)/lb cat]	1119-1183	1208-1246	1683-1703

\*ash recycle test

\*\*addition of Fe<sub>2</sub>O<sub>3</sub> at 1.5% MF coal



### RITSL yield structures (water addition & ash recycle)

run no.	249D	249E	249H**
<b>coal conversion</b> (% MAF cresol sol)	92	89	94
<b>yield*</b> (% MAF coal)			
C <sub>1</sub> -C <sub>3</sub> gas (total gas)	7(18)	6(14)	7(16)
water	14	14	14
C <sub>4</sub> + distillate	53	57	56
resid	1	-4	-4
hydrogen consumption	-5.7	-5.8	-6.3
<b>hydrogen efficiency</b> (lb C <sub>4</sub> + dist/lb H <sub>2</sub> consumed)	9.3	9.9	8.9
<b>distillate selectivity</b> (lb C <sub>1</sub> -C <sub>3</sub> /lb C <sub>4</sub> + dist)	0.14	0.10	0.12
<b>energy content of feed coal rejected to ash conc.</b> (%)	25	30	35
<b>organics rejected to ash conc.</b> (% MAF coal)	21	24	26

\*elementally balanced yield structures

\*\*ash recycle test

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**CATALYTIC**

**RITSL vs ITSL comparison  
subbituminous coal**
**TSL operating conditions**

	249E	246G
run no.	249E	246G
configuration	RITSL	ITSL
catalyst operating mode	batch	batch

**thermal stage**

average reactor temperature (°F)	796	813
inlet hydrogen partial pressure (psi)	2040	2040
coal space velocity [lb/hr-ft <sup>3</sup> (>700°F)]	14	17
solvent-to-coal ratio	1.5	1.8
iron-oxide (% MAF coal)	1.5	2.0
backmixed reactor	yes	no

**catalytic stage**

reactor temperature (°F)	700	625
space velocity (lb feed/hr-lb cat)	1.2	1.0
catalyst age (lb resid/lb cat)	1208-1246*	496

\*based on (lb resid + UC + ash)/lb cat

**RITSL vs ITSL comparison  
subbituminous coal**

**TSL yield structures**

run no.	249E	246G
configuration	RITSL	ITSL
catalyst operating mode	batch	batch
<b>coal conversion (% MAF cresol sol)</b>	89	92
<b>yield* (% MAF coal)</b>		
C <sub>1</sub> -C <sub>3</sub> gas (total gas)	6(14)	9(19)
water	14	11
C <sub>4</sub> + distillate	57	53
resid	-4	1
hydrogen consumption	-5.8	-5.4
<b>hydrogen efficiency (lb C<sub>4</sub>+ dist/lb H<sub>2</sub> consumed)</b>	9.9	9.8
<b>distillate selectivity (lb C<sub>1</sub>-C<sub>3</sub>/lb C<sub>4</sub>+ dist)</b>	0.10	0.18
<b>energy content of feed coal rejected to ash conc. (%)</b>	30	22-24
<b>organics rejected to ash conc. (% MAF coal)</b>	24	21

\*elementally balanced yield structures



## properties of distillate products

distillation cut	wt % of crude	elemental (wt %)					API
		C	H	N	S	O (diff)	
<b>ITSL (run 246)</b>							
naphtha (IBP-350°F)	19.4	83.06	13.23	0.18	0.51	3.02	47.6
distillate (350-650°F)	68.9	86.09	10.80	0.25	0.07	2.79	20.0
gas oil (650°F+)	11.7	88.85	9.23	0.42	0.05	1.45	—
<b>RITSL (run 249F)</b>							
naphtha (IBP-350°F)	31.2	84.47	13.71	0.13*	0.09	1.60	45.6
distillate (350-650°F)	58.5	86.72	11.73	0.53*	0.03	0.99	23.4
gas oil (650°F+)	10.3	88.78	10.68	0.44*	0.08	0.06	—

\*nitrogen by combustion analyzer

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**CATALYTIC**

## run 250

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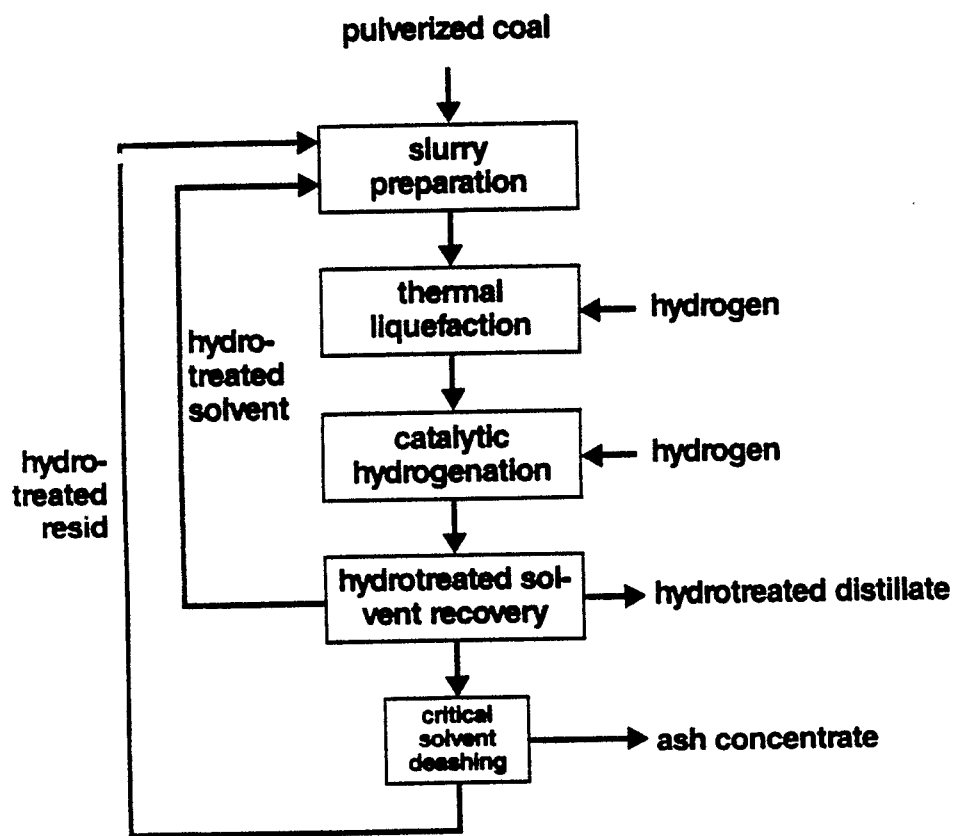
### features

- Illinois no. 6 coal
- CC-ITSL configuration
- catalysts  
dissolver - none  
hydrotreater - unimodal NiMo  
- bimodal NiMo

### results

- good operability
- yields similar to ITSL, higher hydrogen consumption, improved product quality
- good catalyst activity, bimodal catalysts better
- process yields improved by ash recycle

**CC-ITSL**  
**two-stage liquefaction**  
**close-coupled mode**



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**CC-ITSL  
space velocity studies**
**TSL yield structures**

run no.	250C	250D	250E
<b>yield* (% MAF coal)</b>			
C <sub>1</sub> -C <sub>3</sub> gas (total gas)	5(11)	7(12)	6(12)
water	10	10	9
C <sub>4</sub> + distillate	61	64	58
resid	2	-2	7
hydrogen consumption	-5.6	-6.1	-5.7
<b>hydrogen efficiency (lb C<sub>4</sub>+ dist/lb H<sub>2</sub> consumed)</b>	10.9	10.5	10.2
<b>distillate selectivity (lb C<sub>1</sub>-C<sub>3</sub>/lb C<sub>4</sub>+ dist)</b>	0.09	0.11	0.11
<b>energy content of feed coal rejected to ash conc. (%)</b>	24	23	22
<b>organics rejected to ash conc. (% MAF coal)</b>	22	22	19

\*elementally balanced yield structures

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## **1985 accomplishments**

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- **demonstrated RITSL**
  - Illinois and Wyodak coals
  - good operability
  - good catalyst activity
  - basis for close-coupling reactors
- **demonstrated CC-ITSL**
  - Illinois coal
  - good operability
  - tested both unimodal and bimodal catalysts
- **demonstrated improved economics**
  - CC-ITSL
  - ash recycle
- **broadened CSD knowledge**

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## **future work**

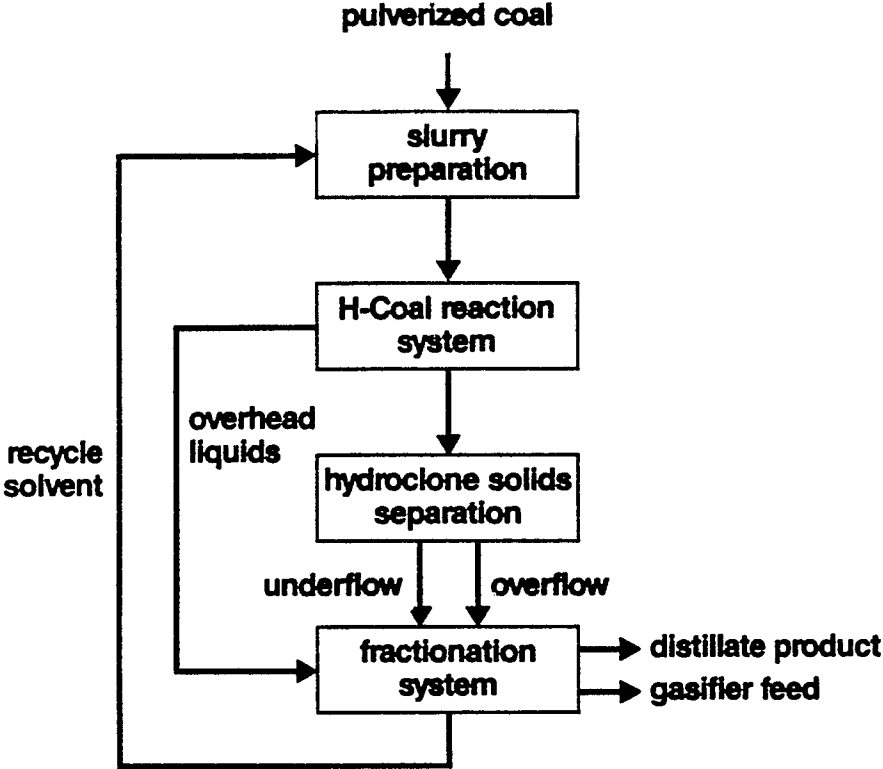
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- close-coupled reactors
    - catalytic-catalytic
    - thermal-catalytic
    - alternate catalysts
    - product slate flexibility
  - process modeling/simulation
  - co-processing
- 

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# H-Coal process

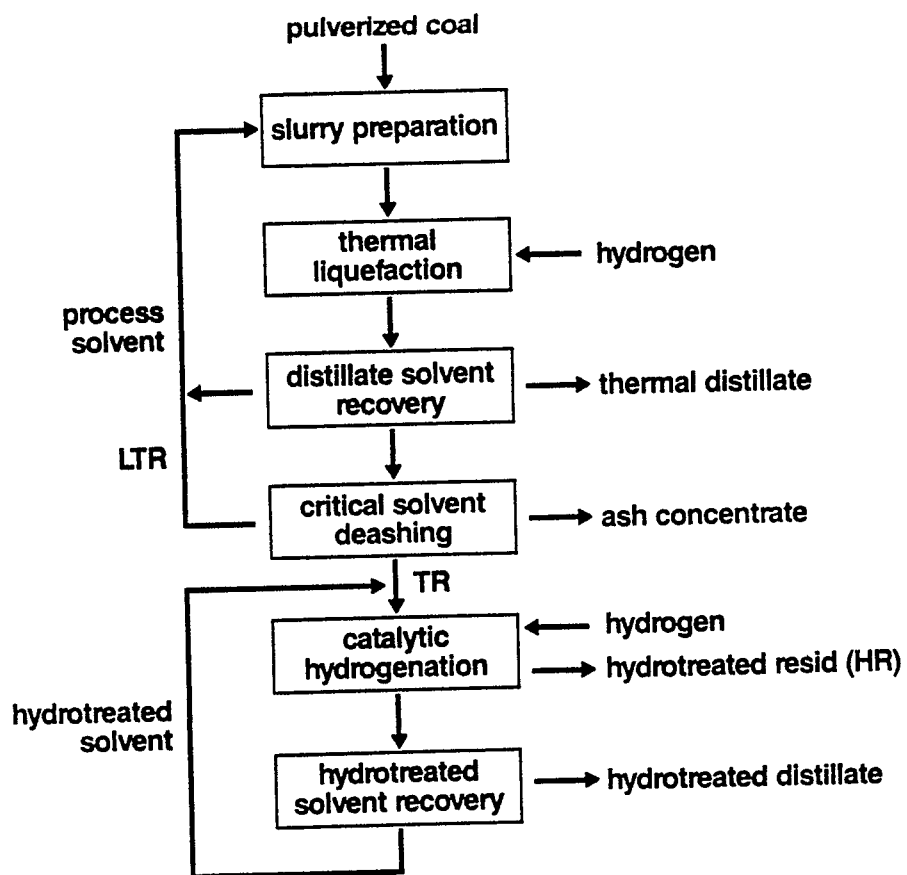


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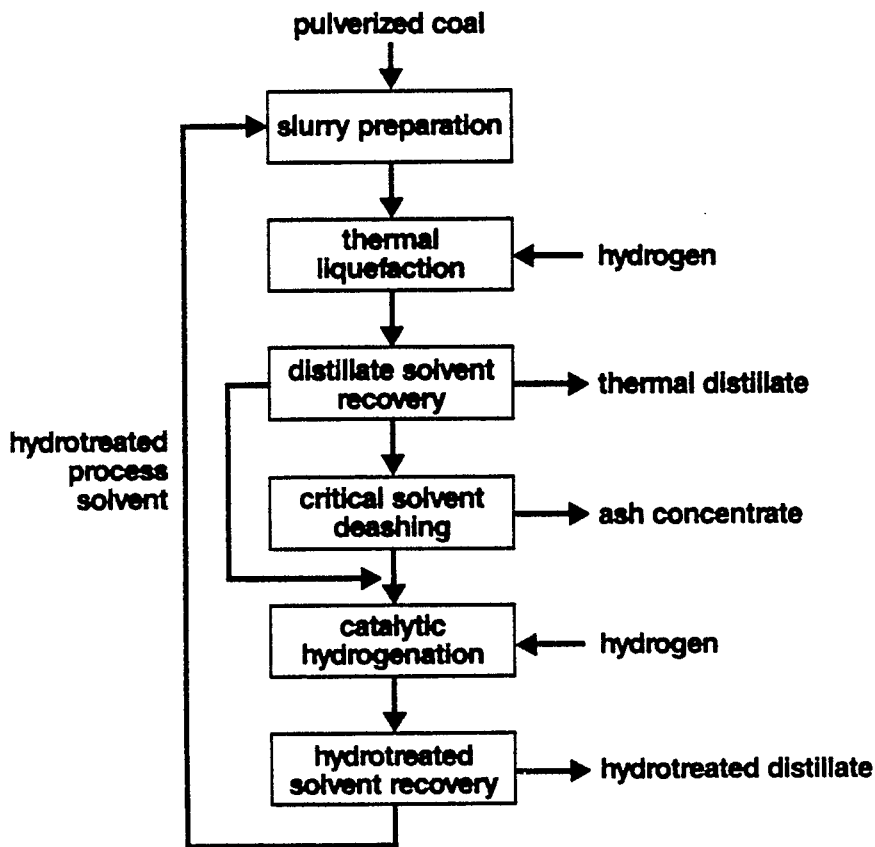


## two-stage liquefaction non-integrated mode (NTSL)



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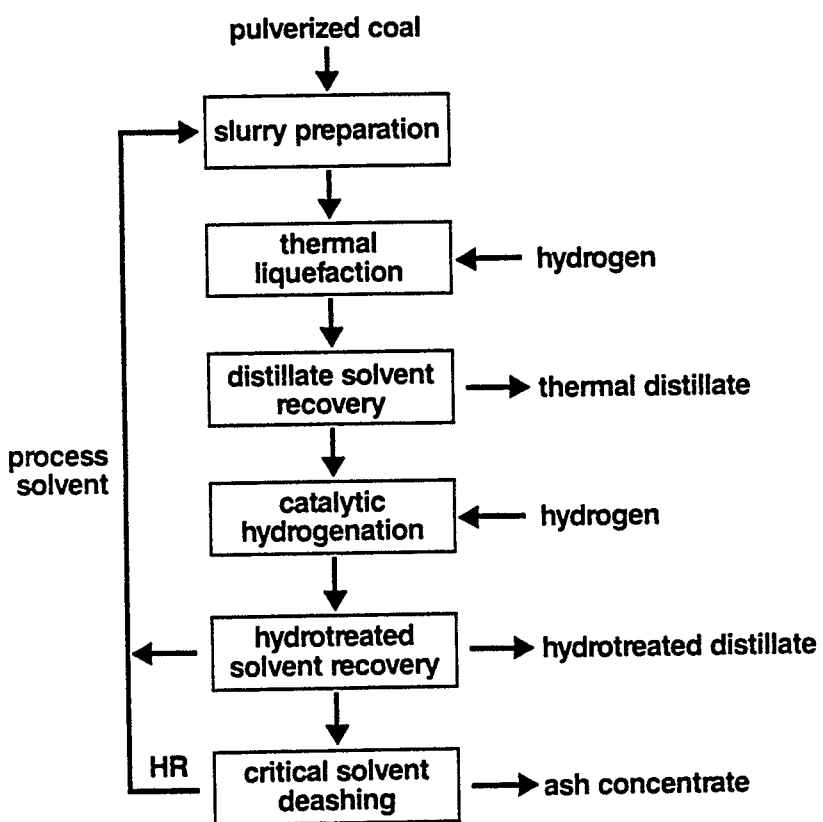
## two-stage liquefaction integrated mode (ITSL)



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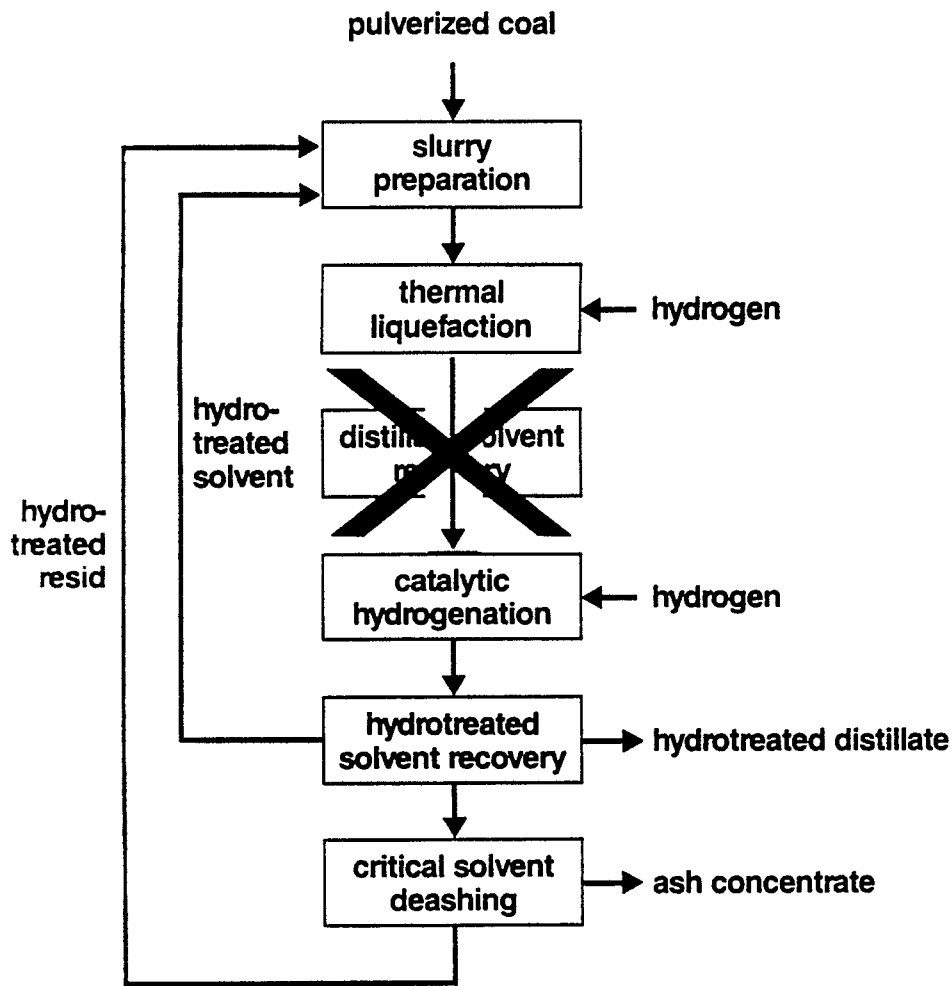
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## two-stage liquefaction reconfigured mode (RITSL)



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**CC-ITSL**  
**two-stage liquefaction**  
**close-coupled integrated mode**



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### relative cost factors

	H-Coal	NTSL	ITSL	CC-ITSL
total plant cost	1.0	1.0	1.16	1.20
total capital required	1.0	1.0	1.16	1.21
operating cost	1.0	1.14	1.45	1.46
annual production cost	1.0	1.07	1.31	1.34
annual production rate	1.0	1.03	1.31	1.43
required product selling price <sup>1</sup>	1.0	1.04	1.00	.93

<sup>1</sup>first year price

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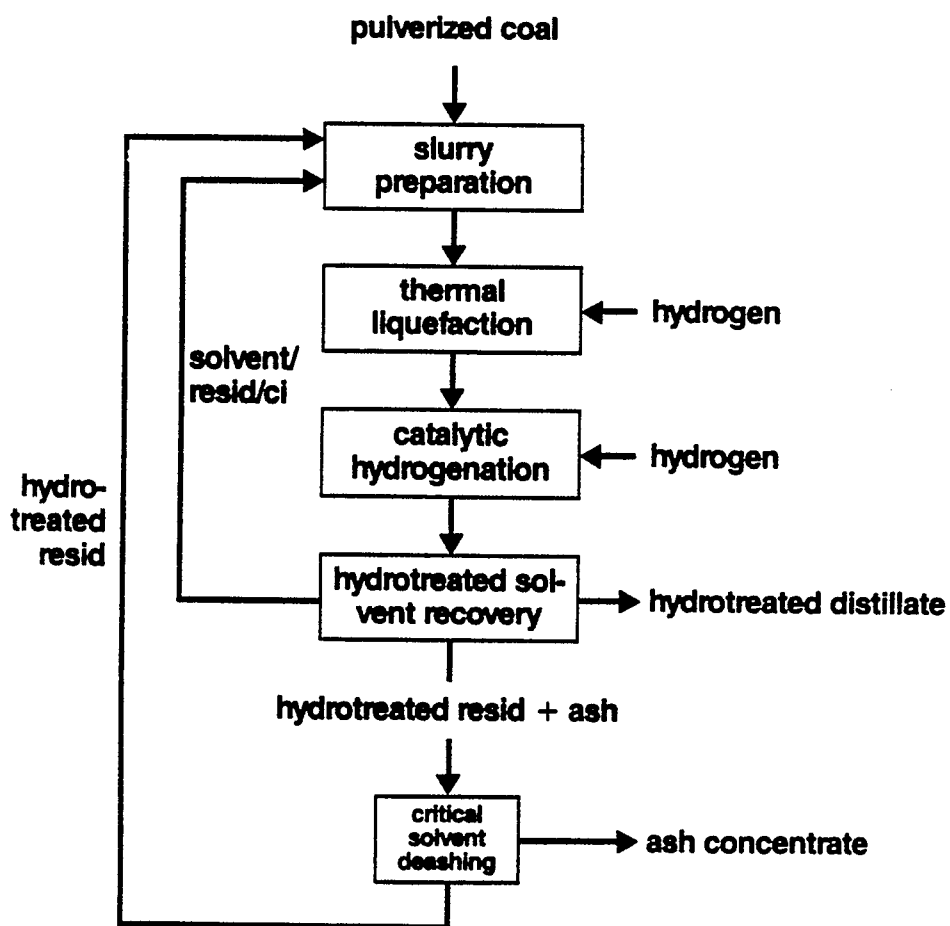


RELATIVE COST FACTORS  
CAPITAL SENSITIVITY

	H- COAL	CCITSL (RUN 247)
TOTAL PLANT COST	1.00	1.10
TOTAL CAPITAL REQUIRED	1.00	1.11
OPERATING COST	1.00	1.35
ANNUAL PRODUCTION COST	1.00	1.23
ANNUAL PRODUCTION RATE	1.00	1.43
REQUIRED PRODUCT <sup>⓪</sup> SELLING PRICE	1.00	0.86

⓪ FIRST YEAR PRICE

# CC-ITSL with ash recycle two-stage liquefaction close-coupled mode



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RELATIVE COST FACTORS  
RECENT DEVELOPMENTS

	H-COAL	CCITSL (RUN 250)	
		HIGH CAPITAL	LOW CAPITAL
TOTAL PLANT COST	1.00	1.20	1.10
TOTAL CAPITAL REQUIRED	1.00	1.21	1.11
OPERATING COST	1.00	1.46	1.35
ANNUAL PRODUCTION COST	1.00	1.37	1.37
ANNUAL PRODUCTION RATE	1.00	1.59	1.59
REQUIRED PRODUCT <sup>⓪</sup> SELLING PRICE	1.00	0.84	0.77

⓪ FIRST YEAR PRICE

UTILIZATION OF HYDROGEN DURING COAL LIQUEFACTION

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## UTILIZATION OF HYDROGEN DURING COAL LIQUEFACTION

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### ABSTRACT

The patterns of hydrogen utilization are determined for a number of different coal conversion conditions. The total uptake of hydrogen is divided into the four categories of gas make, heteroatom removal, change in aromaticity, and cleavage or formation of matrix bonds. Liquefaction temperature strongly influences the extent of hydrogenation of aromatic carbon. Even under significant hydrogen pressure, hydroaromatic compounds underwent net dehydrogenation at temperatures above 400°C. A system comprising water, carbon monoxide, and a basic catalyst was able to hydrogenate coal at 350°C to a greater degree than hydrogen under the same conditions with or without ammonium molybdate added as catalyst. Kinetic experiments with conventional liquefaction feed slurries indicate that tetrahydrofuran and cyclohexane conversions increase with time under low-severity conditions. There is a parallel increase in hydrogen incorporated to break matrix bonds, but the amount incorporated to liberate heteroatoms does not correlate strongly with conversion.

### INTRODUCTION

The transfer and redistribution of hydrogen are among the most important reactions in the liquefaction of coal. The chemistry of reactions involving hydrogen are of interest at several levels. A complete description at the most fundamental level of the basic chemical reactions that liquefaction comprises is not yet available. However, a description at a more general level may still provide valuable insights from the viewpoints of both fundamental chemistry and liquefaction economics. The analytical method used in this work is designed to

give quantitative answers to the question of how much hydrogen is used in each of four categories of reaction in liquefaction. Such information has been obtained as a function of several process variables, such as reaction time, temperature, reducing gas, liquefaction solvent, and the presence or absence of catalysts. The results are useful in guiding strategies for more efficient and effective utilization of hydrogen, and for framing more questions about the mechanism of coal liquefaction that need to be answered at a more fundamental level.

## EXPERIMENTAL

For the experiments reported in Tables 1 and 2, coal liquefaction was conducted in a 0.5-L stirred autoclave. In a typical experiment, 30 to 50 g (maf) of coal ground to pass 60 mesh was charged to the autoclave along with water or coal-derived solvent. When used, the solvent was a distillate cut (240°C-450°C) obtained from operations at the SRC-II pilot plant formerly at Ft. Lewis, Wash. The autoclave was pressurized with the appropriate amount of gas to obtain the desired partial pressure at operating temperature. Heat-up times to liquefaction temperatures were about 45 minutes. The autoclave was held at temperature for the specified time and then rapidly cooled by means of internal water-cooling coils. Grab samples of the off-gas were taken for analysis by gas chromatography as the autoclave was depressurized.

The experiments on the kinetics of coal conversion were conducted in small autoclaves of 42-mL capacity. Heating was achieved by immersion of a bank of five autoclaves in a hot, fluidized sand bath. The time required to reach operating temperature was about six minutes. Cooling was accelerated by immersion in a room temperature fluidized sand bath. Agitation was achieved by oscillation over the top of an arc at about 60 cpm.

The coal was an Illinois No. 6, River King Mine, hvC bituminous coal. The elemental analysis was, on an maf basis, C, 73.7%; H, 5.6%; N, 1.5%; O, 14.8%; S, 4.5%. The ash content was 13.6% on an mf basis.

Coal conversions for products of the 0.5-L autoclave were determined by exhaustive Soxhlet extraction with cyclohexane. Cyclohexane conversions for the products from the 42-mL autoclaves were determined using a pressure filtration technique (1). After exhaustive extraction by cyclohexane, the dried residues were extracted and washed on filter paper with tetrahydrofuran (THF). The THF conversions were based on the dried residue.

## RESULTS AND DISCUSSION

The analytical method used to determine hydrogen utilization divides the total amount of hydrogen incorporated into the organic feed into four categories according to the type of reaction involved (2,3,4). These include (1) the production of light hydrocarbon gases, (2) the removal of heteroatoms, (3) the hydrogenation or dehydrogenation reactions involving changes in aromaticity, and (4) the sum of matrix cleavage reactions and condensation reactions.

The rationale for the analytical approach, and the details of the experimental methods and assumptions have been described (2). Briefly, the analytical method rests on only the organic portion of the feed charged to and removed from the autoclave. Measurement of the material balance for molecular hydrogen is not required. The three pieces of data that must be determined are the following: (1) the change in total hydrogen of the organic components, (2) the change in aromatic carbon, and (3) the loss of organic heteroatoms (O, N, and S). The methods employed are classical elemental analysis, gas chromatography of the C<sub>1</sub>-C<sub>4</sub> products, and determination of aromaticity by <sup>13</sup>C NMR of solids or extracts as called for. The elemental analysis and aromaticity of the feed slurry are calculated as the weighted average of values for the coal and solvent.

To obtain hydrogen utilization numbers, the products of each autoclave run are worked up by exhaustive Soxhlet extraction to obtain soluble and insoluble fractions suitable for analysis by NMR. Methylene chloride was used in these extractions because CD<sub>2</sub>Cl<sub>2</sub> was the solvent of choice for NMR analysis of the soluble portion. Elemental analyses and <sup>13</sup>C aromaticity values are obtained for both solubles and insolubles. Grab samples of the off-gas from the autoclave are taken, and the yield of each hydrocarbon gas is determined by combining the GC analyses with the total amount of gases estimated from the final system pressure. The net loss or gain in total organic hydrogen is available by subtraction of the appropriate elemental analyses. This value for the total change is then divided into the four separate categories. The amount incorporated into the liquid products by C<sub>1</sub>-C<sub>4</sub> gas formation is obtained from the calculated volume of off-gas and its determined hydrocarbon gas content. Two atoms of hydrogen are assumed to be incorporated for every molecule of gas released. The amount incorporated by removal of heteroatoms is determined by the net loss of O, N, and S. In these experiments, it is mainly loss of O. It is assumed that one hydrogen is incorporated for every heteroatom lost.

The change in aromaticity is obtained by combination of the NMR data on the solids and on the methylene chloride extract of the product. One hydrogen is incorporated (or lost) for every decrease (or increase) of one aromatic carbon. The number of hydrogens incorporated by matrix cleavage reactions or given up by condensation reactions is calculated as the difference between the total change in hydrogen and the sum of changes in the other three categories. Of the four categories, the largest error resides in the matrix cleavage values. This value rests in part on the total organic hydrogen in the feed coal. The hydrogen in coal was determined by the standard ASTM procedure. Nonetheless, the "dry" coal used in this determination may still contain hydrogen in the form of water that is released only under more severe drying conditions such as encountered during liquefaction. If there was loss of residual water from the "dried" coal, it would translate into opposing systematic errors in the absolute values for matrix cleavage and heteroatom removal. However, the relative trends for matrix cleavage values to increase or decrease for a particular coal over a series of experiments would not be affected by this systematic error. The possibility of this systematic error aside, the random errors of the analytical methods are estimated to be about  $\pm 1$  H/100 C. The results of the duplicate liquefaction experiments have usually been within this range. The hydrogen utilization values are all tabulated on the basis of hydrogens per 100 carbons in the organic feed, which includes both coal and the organic solvent (when used). Coal conversion values were measured for comparison with hydrogen utilization data in parallel experiments using the same liquefaction conditions.

#### Catalyst and Temperature Effects

Liquefaction yields are well known to be strongly influenced by the reaction temperature and the presence of added catalysts. To survey the effects of these two variables on hydrogen utilization, a small set of experiments were run at three temperatures using two commonly employed catalysts. The results are gathered in Table 1. Coal conversions were also obtained for comparison. The conversions were measured by cyclohexane extraction to obtain a rough measure of distillate yields.

Several interesting comparisons can be made among the data in Table 1. The catalysts used (ammonium molybdate and two tin compounds) were thought to act in liquefaction by different means (5). Ammonium molybdate is noted for hydrogenation activity, but the tin compounds are not. However, differences in the hydrogen utilization data between ammonium molybdate and tin tetrachloride were



not striking. Tin disulfide was not effective. It is apparently much less active than the chloride-containing catalyst.

TABLE 1. Coal Conversion and Hydrogen Utilization for Catalyzed and Non-Catalyzed Liquefaction.

Catalyst	T., °C	Conv.	Heteroatom Removal	Hydrogenation	Matrix Cleavage <sup>1</sup>	Gas Make	Total <sup>2</sup>
AmMo	375	18	1	2	2	0	5
SnCl	375	21	0	4	0	0	4
AmMo	400	37	2	0	2	0	4
None	425	35	2	-5	5	1	3
AmMo	425	54	2	-4	11	2	11
SnCl	425	51	1	-4	10	2	9
SnS	425	NA	2	-6	2	1	-1

Note: All liquefactions are under approximately 2000 psia hydrogen partial pressure at operating temperature, using 2 parts solvent and 1 part maf Illinois No. 6 coal. Reaction time was 15 minutes. Catalyst loading was 1.5% of metal based on maf coal. Molybdenum was added as ammonium molybdate, AmMo. Conversion values are in wt% of maf coal, determined from dry weight of residue after exhaustive cyclohexane extraction.

<sup>1</sup>Determined by difference.

<sup>2</sup>All utilization numbers in hydrogens per 100 carbons in feed slurry.

Temperature has a large effect on the pattern of utilization. There is a change again from net hydrogenation to net dehydrogenation between 375°C and 425°C. No change in aromaticity was observed at 400°C. Appropriate amounts of hydrogen were charged to the autoclave to maintain its partial pressure at temperature at roughly 2000 psia in all cases. The direction of the change is expected because at equilibrium, higher temperatures generally favor the formation of aromatic compounds from hydroaromatic compounds by release of hydrogen. The general trend from hydrogenation to dehydrogenation as the liquefaction temperature is raised above 400°C was also observed earlier for uncatalyzed reactions (4).

The addition of the active catalysts at 425°C had a large effect on the amount of hydrogen consumed during the cleavage of matrix bonds. The method measures net hydrogen utilization without regard to the details of the chemical mechanism. Thus, from these data alone, it cannot be said whether the increase in hydrogen use is due to promotion of bond cleavage directly or to the prevention of condensation reactions between reactive fragments created by simple thermal bond

scission. At 375°C, there was little net change in matrix bonds in the presence of ammonium molybdate, and no net change in the presence of tin tetrachloride. Of course, because only net changes are measured, this does not necessarily mean that matrix bond cleavage did not occur. It may be that cleavage reactions are nearly balanced by condensation reactions.

The amount of hydrogen consumed to remove heteroatoms is relatively small, as expected under mild liquefaction conditions. As was the case with non-catalytic conversions, almost all of this hydrogen is used in the removal of oxygen. There is essentially no change in nitrogen content and only a small reduction of organic sulfur.

There is a considerable increase in coal conversion with increasing liquefaction temperature. The presence of either ammonium molybdate or tin tetrachloride also makes a large difference in conversion at the one temperature where comparison with an uncatalyzed reaction is possible.

Of all the hydrogen utilization values, the general trend of coal conversion most strongly follows that of matrix bond cleavage. This result is entirely consistent with the simple idea that more bonds must be broken to increase the yield of lower molecular weight products.

Hydrogen utilization data may be used to recognize patterns of response to changes in process variables. It is particularly interesting to study the relationship between hydrogen utilization and conversion as a single process parameter is changed. For example, utilization data selected from Table 1 for liquefaction with ammonium molybdate catalyst are plotted in Figure 1 as a function of cyclohexane conversion. In this subset of experiments, all variables were held constant except the liquefaction temperature, which increased from 375°C to 425°C. A pattern of change in hydrogen utilization is thus given as cyclohexane conversions are increased by means of raising the temperature. A significant increase in conversion is brought about by increasing the temperature from 375°C to 400°C without much change in total hydrogen consumption. A further 25°C increase in temperature brings about a still higher conversion, but hydrogen consumption also jumps markedly. The largest increase is in the cleavage of matrix bonds, although gas make also becomes significant for the first time. At the higher temperature, hydrogenation values are now negative. It is reasonable to expect that hydrogen demanded by reactions in the other three categories is now partially supplied by dehydrogenation of the organic feed. Thus, higher tem-

peratures bring about greater conversion, but the total organic product becomes more aromatic in character. A similar trend to higher aromaticity in liquefaction products generated above 400°C was seen earlier for experiments without catalyst (4). Quantitative data of this sort may be of some assistance in guiding strategies to improve efficiency in using hydrogen. For example, the present case might be used to justify exploration of the strategy of conducting hydrogenation at lower temperatures and promoting cleavage reactions in a subsequent step at higher temperature.

#### Aqueous Systems

Water is a chemically suitable medium for the liquefaction of coal under appropriate conditions (6). Experiments using water in place of the usual organic solvent have been of value in providing examples of liquefaction chemistry quite different from that found in more conventional systems. Some aspects of this chemistry are revealed by analyzing the products in terms of hydrogen utilization. In some respects, interpretation of the data obtained with water is simplified because all of the organic products originate from the coal.

Table 2 contains data for experiments in which 50 g of coal (maf) was mixed with 100 g of water. This survey includes experiments at either of two temperatures, and using several catalysts. Hydrogen, carbon monoxide, or nitrogen were used to provide a range of reducing atmospheres.

Many of the hydrogen utilization values from experiments using water are larger than those using organic solvent reported in Table 1. If the speculation that coal accounts for the majority of the reactions using hydrogen when organic solvent is present is accepted, then the increase in the absolute magnitude of the utilization values is easily understood. The organic solvent may act as a diluent that reduces the observed amount of hydrogen used or given up per 100 carbons of the total organic feed. In water, however, all of the carbon is associated with the coal, thus resulting in observation of larger changes. Aside from this dilution factor, there seems to be a general trend for coal to give up hydrogen more readily by dehydrogenation and condensation reactions in water than does the total mixed feed of coal and recycle solvent.

In water, temperature is again a major determinant of the pattern of hydrogen utilization. At 400°C, there is an overall net loss of hydrogen by coal. Generally, the loss is split between dehydrogenation reactions and condensation

TABLE 2. Hydrogen Utilization for Liquefaction in Water.

T., °C	Catalyst <sup>1</sup>	Pressure <sup>2</sup> , psia	Time, min	Heteroatom Removal	Hydrogenation	Matrix Cleavage	Gas Make	Total <sup>3</sup>
400		750	15	4	-9	-2	2	-5
400		800 (H <sub>2</sub> )	20	3	-11	-5	1	-12
400	KOH	800	20	6	-7	-7	2	-6
400	KOH	800	60	7	-6	-5	2	-2
400	Na <sup>+</sup> HCOO <sup>-</sup>	730	20	6	-12	-5	2	-9
350		1000	120	5	-1	-1	0	2
350		1000	60	3	-2	0	0	1
350	KOH	1000	60	3	4	2	0	9
350	AmMo	1000	60	3	-1	-1	0	1
350		1000 (H <sub>2</sub> )	60	2	-5	-8	0	-11
350		1000 (N <sub>2</sub> )	60	4	-7	-7	0	-10

<sup>1</sup>Catalyst loadings were 1% by weight of KOH or sodium formate, or 0.4% of ammonium molybdate.

<sup>2</sup>Pressure was measured at room temperature. Reducing gas used was CO unless otherwise indicated.

<sup>3</sup>Hydrogen utilization values are in hydrogens per 100 carbons in coal.

reactions. The latter are reflected as negative values for matrix cleavage. In contrast, at 350°C under CO, there is little change in total hydrogen in the absence of catalyst. In the presence of KOH, there is a sizable uptake of hydrogen.

The type of reducing gas has a large influence at 350°C. With either H<sub>2</sub> or N<sub>2</sub> replacing CO, there is again a large net loss of hydrogen by coal. The loss is accounted for by both dehydrogenation and condensation, as it was at 400°C.

Other general trends are also apparent. Gas make is virtually nil at 350°C. The loss of heteroatoms, which is almost totally due to loss of oxygen in these experiments, is not as great at 350°C as at 400°C. The exception to this observation is the higher value at 350°C for the one experiment run for 120 minutes. Thus, the rate of loss may be slower at the lower temperature.

The role of catalyst is also closely related to liquefaction temperature. Although the data are incomplete, addition of KOH markedly increases the total amount of hydrogen taken up by coal at 350°C. At 400°C, the difference on addition of KOH is mostly associated with an increased loss of hydrogen by condensation reactions.

#### Kinetics of Liquefaction and Hydrogen Utilization

Kinetic studies have provided many interesting insights into the chemistry of liquefaction. Comparison of the kinetics of coal conversion to data for the utilization of hydrogen provides additional information about the time course of the separate categories of hydrogen reaction. The objective of the initial experiment was to explore the kinetics of the primary dissolution of coal at a moderate reaction temperature. A series of experiments were carried out in small (42-mL) shaking autoclaves at 380°C. Reaction times were varied from zero time at temperature to 60 minutes. A rather conventional feed slurry (solvent/Illinois No. 6 coal = 2/1, 1200-psig H<sub>2</sub> at room temperature) was chosen as a trial case. Catalysts, either ammonium molybdate or tin tetrachloride, were added at the level of 0.1% metal on maf coal in two of three cases. Cyclohexane and THF conversions are shown as a function of time in Figure 2.

The data in Figure 2 show that both THF and cyclohexane conversions increase with reaction time. Differences between catalyzed and uncatalyzed liquefactions are not apparent for THF conversions. The use of the tin catalyst appears to

slightly increase the cyclohexane conversion in most cases. In general, the effect of added catalysts on liquefaction yields at the relatively mild temperature chosen for these initial studies was less than anticipated.

The time course of hydrogen utilization for these experiments is shown in Figure 3. Differences between catalyzed and uncatalyzed reactions are now more apparent, particularly for total hydrogen incorporation. The incorporation for the uncatalyzed case gradually increases with time and eventually approaches the value for the catalyzed liquefactions. In general, the tin-catalyzed liquefaction resulted in the greatest hydrogen incorporation, in parallel with the somewhat greater cyclohexane conversion. The catalyzed uptake of hydrogen seems to be delayed until after ten minutes at reaction temperature. This pattern is also evident in the category for matrix cleavage. The values in some cases are negative in the first ten minutes. This may reflect a period during which certain condensation reactions are prominent. Following the possible exhaustion of the most probable condensation reactions, the slower process of bond cleavage then begins to dominate the balance between cleavage and condensation. Net incorporation of hydrogen is then the result. These speculations will be used to guide our further experimentation, but the correlation of conversion and hydrogen utilization data, however useful, is still insufficient to establish a cause and effect relationship. Further work is aimed at establishing the generality of the trends observed in the kinetic experiments.

#### ACKNOWLEDGMENTS

We are indebted to R.F. Sprecher for the NMR analyses essential to this work, to W.L. Lipinski for assistance with the autoclave liquefactions, and to B.M. Thames for assistance with the analysis of the liquefaction products.

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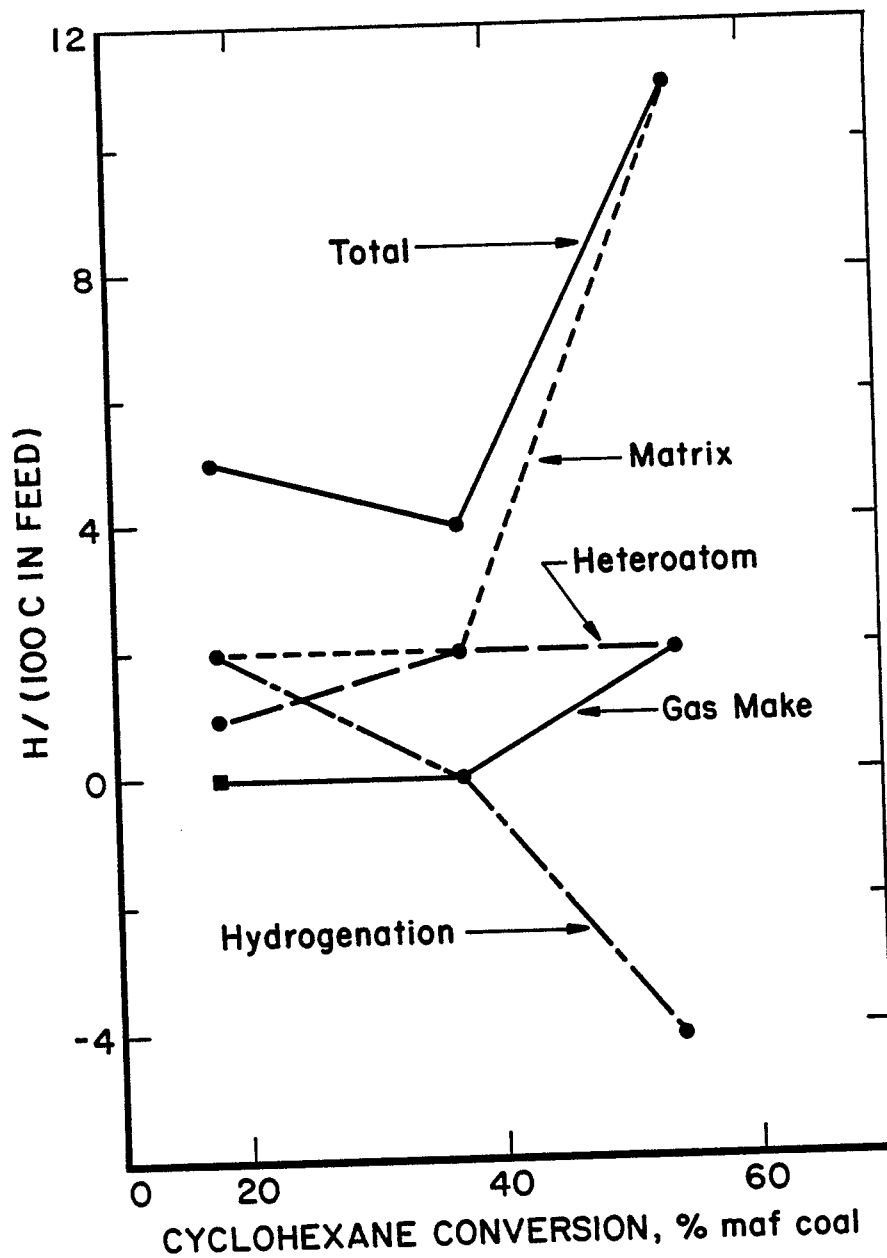


Figure 1 - Hydrogen Utilization for Ammonium Molybdate Catalyzed Conversions at 375°, 400°, and 425°C.



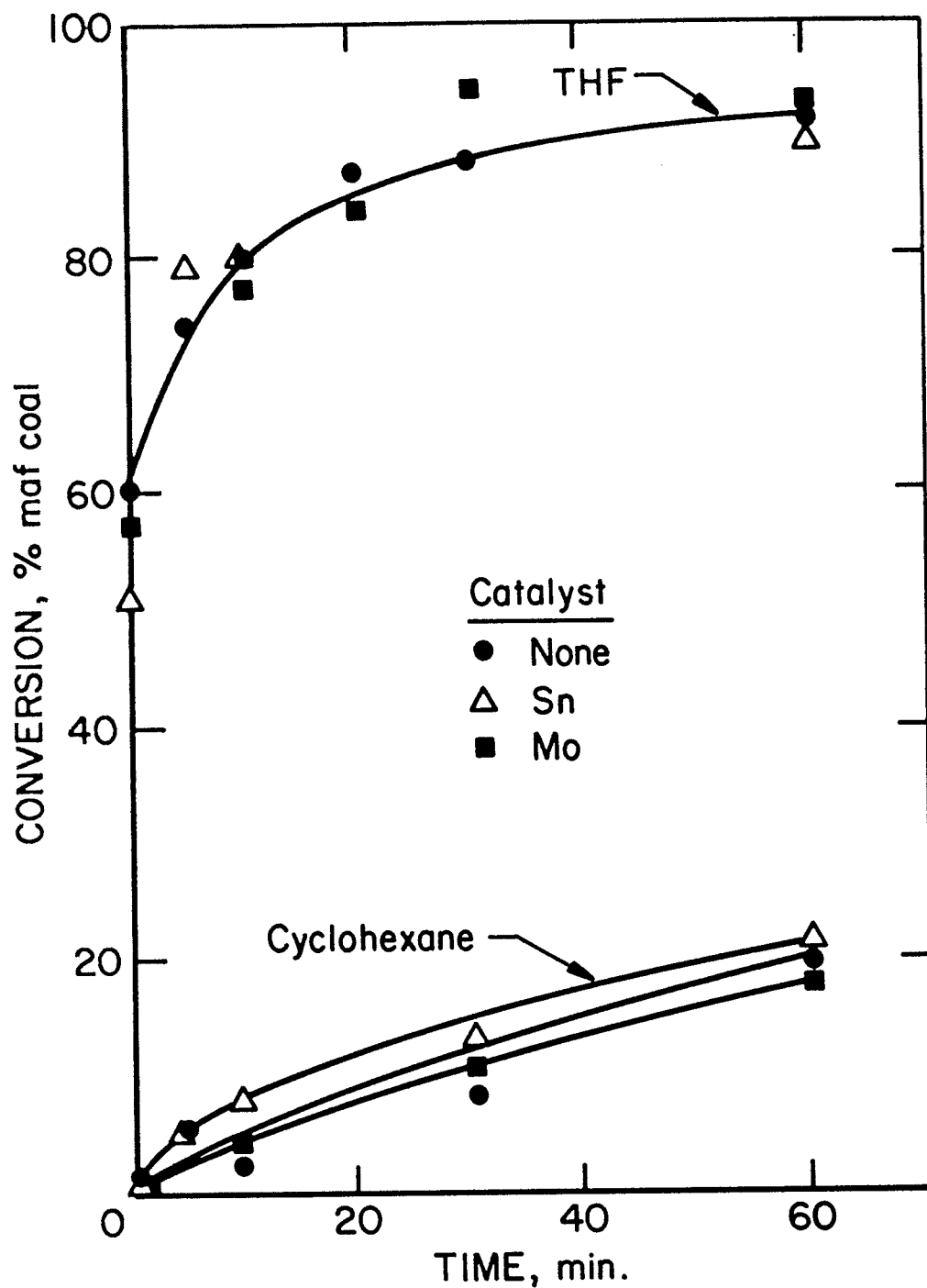


Figure 2 - Conversion of Illinois No. 6 coal at 380°C.

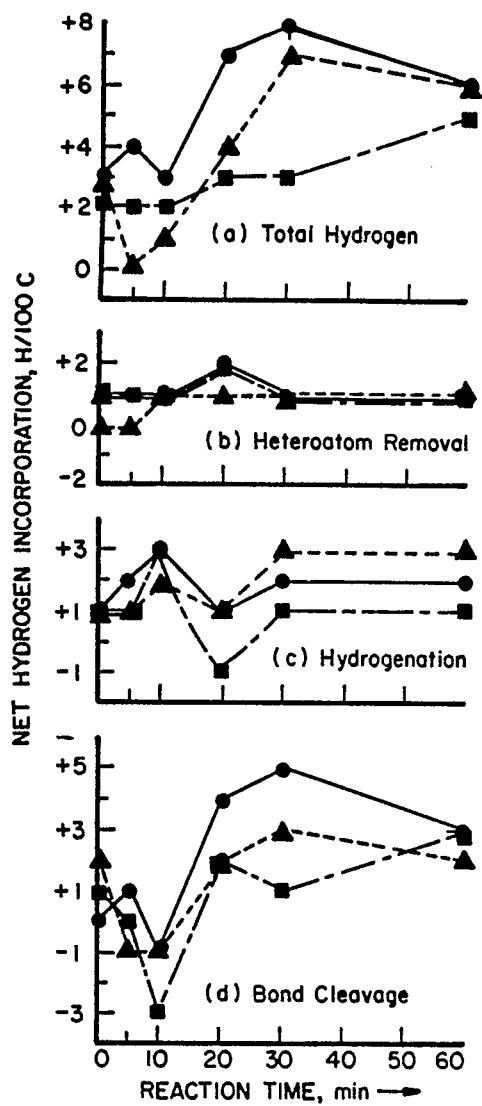


Figure 3 - Hydrogen Utilization as a Function of Reaction Time.

- — Sn Catalyzed
- ▲ - - - Mo Catalyzed
- - - - Uncatalyzed

TWO-STAGE LIQUEFACTION COAL DERIVED LIQUID  
AS A COMBUSTION TURBINE FUEL

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## ABSTRACT

The objective of the Integrated Two-Stage Liquifaction (ITSL) coal derived liquid fuel laboratory test program was to evaluate the emissions and combustor performance characteristics of a W251AA combustor when burning the ITSL coal-derived liquid fuel, and thus determine the acceptability of the test fuel as an electric utility combustion turbine fuel. The ITSL fuel was found to be an acceptable coal-derived liquid fuel. The chemical and physical properties of the ITSL CDL fuel were determined. The trace metals, such as sodium, potassium, vanadium, etc., are low and within values presently allowable in fuel oil specifications. The burner performance factors (pressure drop and exit temperature pattern factor) on the CDL test fuel did not differ significantly from those of the baseline No. 2 fuel. The efficiencies when burning either fuel were generally high (99+%). Evaluation and comparison of the ITSL and baseline No. 2 combustor wall temperature data, show the increase in wall temperature (above No. 2 baseline data) to be consistent with expectations. The ITSL test data on wall temperatures complement and extend the CDL data base for evaluation of coal-derived liquid fuels. The laboratory wall temperature data compared well with previous test results. Emissions were measured over an equivalent load range of 30% to 100% engine base load. The increase in the measured  $\text{NO}_x$  emissions with increasing combustor temperature rise (load), or outlet gas temperature, was observed. The usual reduction of  $\text{NO}_x$  with water injection into the combustion chamber was also observed. Other emissions, such as CO, UHC, O<sub>2</sub>, and CO<sub>2</sub> for the ITSL CDL fuel generally followed the usual characteristics with load.

## 1. INTRODUCTION

As an extension of EPRI's overall program to determine the suitability of using coal-derived liquids as utility combustion fuels, Contract RP2112-5, Evaluation of Coal Liquids as Utility Combustion Fuels, was expanded in scope to include laboratory testing of the Integrated Two-Stage Liquifaction (ITSL) coal derived liquid (CDL) fuel. This conference paper reports the results of work performed by the Westinghouse Electric Corporation, Combustion Turbine Engineering Department, Generation Technology Systems Divisions, under the expanded scope. The added laboratory testing was a logical extension of earlier testing of CDL fuels in a utility gas turbine power plant to assess the effects of burning coal liquids on gas turbine systems. (1, 2)\*

The objective of the laboratory test program was to evaluate the emissions and combustor performance characteristics of a W251AA combustor when burning the ITSL coal-derived liquid fuel, and thus determine the acceptability of the test fuel as an electric utility combustion turbine fuel.

The ITSL fuel is produced in limited quantities in the Wilsonville, Alabama, Advanced Coal Liquidfaction Unit operated by Catalytic, Inc., under contract to Southern Company Services. The Wilsonville coal liquifaction program is sponsored by EPRI, U.S. Department of Energy and Amoco Corporation. The production process incorporates two stages of hydrogenation. The test fuel from the Wilsonville plant was a heavy distillate product with a high distillation range (95% at 865°F). Its hydrogen content of 10.91%, by weight, is comparable to about 13% for No. 2 fuel oil, 10.5% for H-Coal<sup>®</sup>, and 10% for Exxon Donor Solvent (EDS) fuels.

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\*References are identified by (X) and are given in Section 6.

<sup>®</sup>Registered trademark.

## 2. COMBUSTION TEST SYSTEM

The ITSL CDL combustion tests were run in the Westinghouse Combustion Turbine Development Center located at Concordville, Pennsylvania. The test combustor was installed in the facility test rig shown in Figure 2-1. The rig is configured to simulate a sector of an engine. Inlet and exit instrumentation are identified on the figure. The combustor pressure rakes are located at the diffuser exit; the air inlet temperature is measured within the rig inlet chamber. Air and fuel flow are metered upstream of the rig. The exit gas temperature and emissions sampling rake locations are shown on the figure.

The W251AA test combustor installed in the rig is shown in Figures 2-2 and 2-3. The combustor configuration was the same as that field tested on H-Coal and EDS coal-derived liquid (CDL) at the Philadelphia Electric Company's (PECO's) Richmond Station at Philadelphia, Pa. in 1982-1983(1). Figure 2-2 shows the modifications required to fit within the test rig. The figure also shows the wall thermocouple locations for the ITSL fuel test program. Ring 0 through 5, inclusive were instrumented as was the PECO field test combustor. Figure 2-3 is a photograph of the instrumented W251AA test combustor.

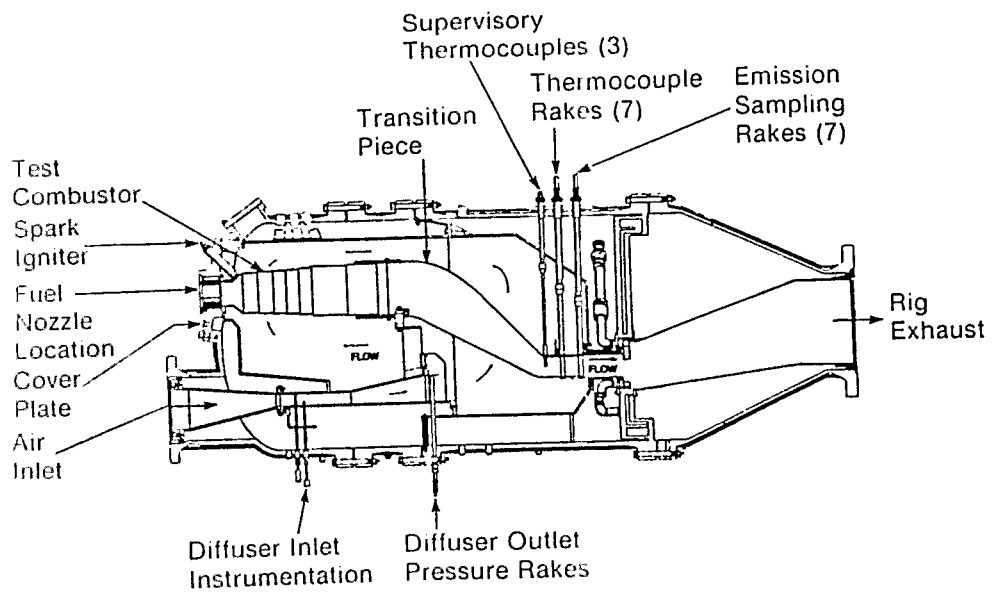


Figure 2-1. Combustor Test Rig

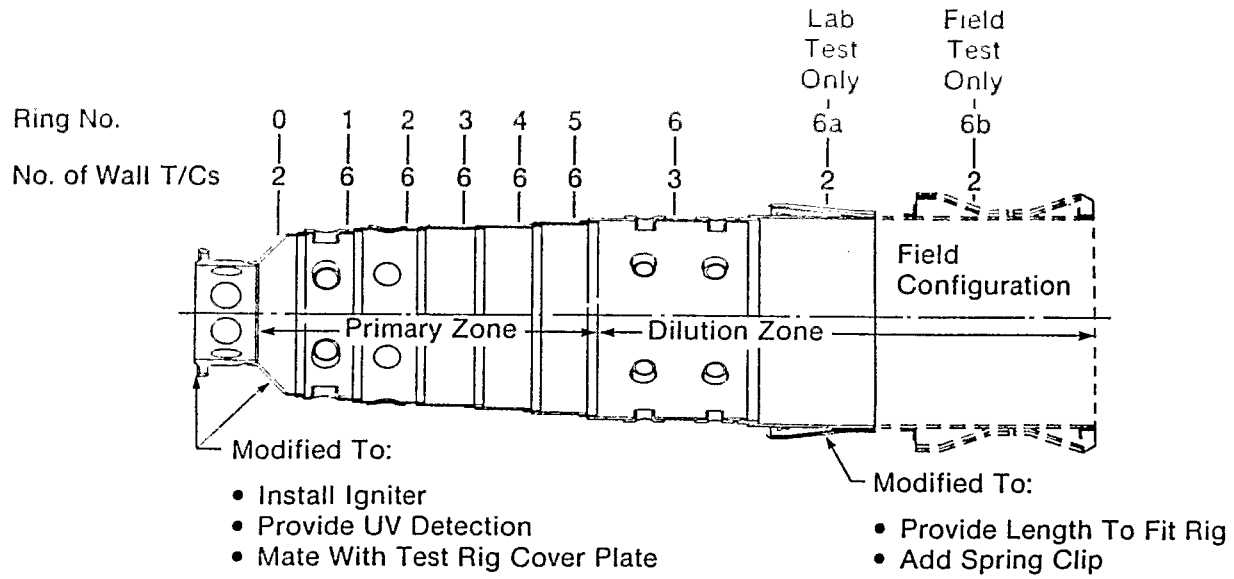


Figure 2-2. W251AA Test Combustor With Wall T/C Locations



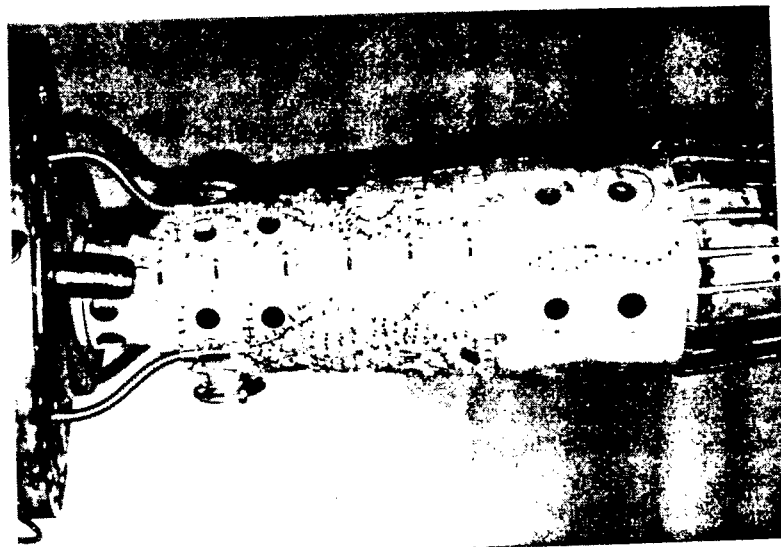


Figure 2-3. W251AA Test Combustor

### 3. FUEL CHARACTERIZATION

The ITSL CDL fuel, was fully characterized. The chemical and physical properties of the fuel were obtained using appropriate ASTM procedures. The resulting data are presented in Tables 3-1 through 3-3. The tables include the properties for H-Coal and EDS CDL liquids, burned in the W251AA engine during field tests (1), for comparison purposes.

The results of the fuel analyses indicated the fuel to be fully acceptable as a combustion turbine fuel. The trace metals, such as sodium, potassium, vanadium, etc., of concern from the high temperature corrosion aspect of the turbine vane and blade materials, are within values presently allowable in combustion turbine petroleum fuel oil ASTM specifications. The viscosity vs. temperature characteristic of the ITSL test fuel was such that the fuel was heated to about 110°F at the combustor nozzle to assure proper fuel atomization in the primary combustion zone of the burner.

Table 3-3, Fuels Distillation Characteristics, shows the ITSL CDL has a high boiling temperature range when compared with typical No. 2 distillate and H-Coal and EDS CDL fuels. The initial boiling point (IBP) is 375°F, and is comparable to the IBP of 360°F, 320°F, and 422°F for No. 2 distillate, H-Coal, and EDS CDLs respectively. The final boiling point (FBP) of 890°F for the ITSL CDL is much higher (84 to 286°F) than the other fuels. This characteristic is considered to be a unique property of the ITSL (heavy distillate) test fuel when compared with the H-Coal (light distillate) and the EDS (full range distillate) CDL fuels. The high FBP appeared to cause no difficulty in fuel handling or burning of the test fuel.

The laboratory fuel forwarding systems, the fuel heating system, and the fuel flow control and metering systems operated well on the ITSL CDL fuel. There was no indication that the test fuel could not be handled by the combustion turbine fuel forwarding and control systems, with appropriate sealing and gasket material changes, if required. Long term stability and storage problems, if any, with the ITSL CDL fuels were not investigated during this experimental program.

Table 3-1

## FUELS PHYSICAL/CHEMICAL PROPERTIES

Fuel:	No. 2 Distillate Typical	ITSL Heavy Distillate 12/10/85	H-COAL Light Distillate 12/13/82	EDS Full Range Distillate 3/17/83
Sample Date:				
Viscosity:				
SSU/°F	42.0/ 65 36.5/100 32.5/150	163.7/ 60 64.9/100 42.5/150	38.0/ 70 34.5/100 32.5/125	52.5/ 72 44.0/100 39.0/120
Specific Gravity				
SPG/°F	0.8510/ 65 0.8400/100 0.8270/150	0.9552/ 60 0.9405/100 0.9218/150	0.9295/ 60 0.9170/100 0.8940/150	0.963/ 63 0.948/100 0.941/120
	<u>°F</u>	<u>°F</u>	<u>°F</u>	<u>°F</u>
Flash Point	195	268	205	230
Fire Point	200	291	215	238
HHV Btu/lb	19113	18682	17647	18273
	<u>%V</u>	<u>%V</u>	<u>%V</u>	<u>%V</u>
Sediment & Water	<0.05	0.08	<0.05	0.25
Water	N.D.	0.05	N.D.	N.D.
Composition	<u>% Wt</u>	<u>% Wt</u>	<u>% Wt</u>	<u>% Wt</u>
Carbon	86.74	88.17	86.24	87.02
Hydrogen	13.25	10.91	10.48	9.97
Nitrogen	0.02	0.13	0.41	0.17
Oxygen	0.69	<0.5	2.75	1.12
Sulfur	0.027	0.03	0.057	0.035
	<u>ppmw</u>	<u>ppmw</u>	<u>ppmw</u>	<u>ppmw</u>
Ash	<0.5	<100	51	6

Note: N.D. = Not Detected

Table 3-2  
 FUELS TRACE METAL CONTENT

Fuel: Sample Date:	No. 2 Distillate Typical	ITSL Heavy Distillate 12/10/85	H-COAL Light Distillate 12/13/82	EDS Full Range Distillate 3/17/83
Trace Metal	ppmw	ppmw	ppmw	ppmw
Sodium	0.020	<0.1	0.044	<0.02
Potassium	N.D.	<0.1	0.024	0.03
Vanadium	0.20	<0.2	1.00	<0.19
Calcium	N.D.	<0.02	0.100	0.06
Lead	0.060	<0.1	0.060	N.D.
Zinc	0.012	0.3	0.060	0.01
Cadmium	N.D.	<0.02	N.D.	N.D.
Nickel	N.D.	0.4	N.D.	N.D.
Iron	0.50	1.64	28.00	3.4
Manganese	0.07	0.04	0.20	N.D.
Magnesium	0.01	<0.02	0.014	0.025
Copper	N.D.	<0.02	0.28	N.D.
Chromium	<0.050	<0.02	<0.050	N.D.

Note: N.D. = Not Detected.

Table 3-3  
FUELS DISTILLATION CHARACTERISTICS

Method of Analysis	Air Distillation ASTM D-86		Vacuum Distillation ASTM D-1160	
	No. 2 Distillate Typical	ITSL Heavy Distillate 12/10/85	H-COAL Light Distillate Typical	EDS Full Range Distillate Typical
Fuel: Sample Date:	°F	°F	°F	°F
<u>%V</u>				
IBP	360	375	320	422
5%	---	460	380	---
10%	420	480	400	422
20%	450	510	410	433
30%	480	540	420	449
40%	500	565	425	475
50%	520	585	435	542
60%	540	615	445	549
70%	560	640	450	610
80%	580	695	470	668
90%	610	775	480	745
95%	---	865	---	806
FBP	660	890	520	806
% Recovery		97		
% Residue	<0.5	2	<0.1	<0.1
% Loss		1		

#### 4. COMBUSTION TEST RESULTS AND COMPARISONS WITH PREVIOUS DATA

The combustion tests run to evaluate the ITSL CDL fuel are outlined in Table 4-1. The test conditions were selected to simulate the W251AA engine conditions during field operation at PECO(1).

Table 4-1  
COMBUSTION TESTS

Two test series

- Baseline No. 2 fuel oil
- ITSL CDL fuel

Equivalent engine load conditions of test series

- 100%, 75%, 50%, 30%
- Without and with water injection
- Water-to-fuel injection ratios from 0 to approximately 1.

Test conditions simulating engine operating environment

- Air flow of 36.2 lb/sec
- Air inlet temperature of 623°F
- Combustor pressure level of 148.4 psia.

Approximate combustor temperature rise vs. % load

<u>Load %</u>	<u>Temperature Rise °F</u>
100	1180
75	990
50	800
30	715

Tests on No. 2 fuel oil were made to establish the baseline combustion characteristics, as was done during the W251AA field testing. These baseline tests were followed by a test series burning the ITSL CDL fuel. In each series, the combustor load condition and the water injection into the combustor (to study reduction in thermal  $\text{NO}_x$ ) were the principal variants. The test conditions were

chosen to provide equivalent data to that obtained during the field tests on H-Coal and EDS CDL fuels. In this manner the laboratory test data, in conjunction with the field data, would provide the data base to determine the acceptability of the ITSL as a combustion turbine fuel.

#### Combustion Performance

The combustor performance data, relative to the baseline No. 2 fuel operation, shows the ITSL fuel to be fully acceptable as a utility gas turbine fuel from a combustion performance view point. The burner performance factors on the CDL test fuel did not differ significantly from those of the baseline No. 2 fuel. The efficiencies when burning either fuel were high (99+%) from the equivalent of 30% to 100% of engine baseload operation without water injection, and from 75 to 100% with water injection. The turbine temperature pattern factor parameter values,  $(T_{\max} - T_{\text{avg}})/(T_{\text{avg}} - T_{\text{inlet}})$ , were low, and ranged between 0.067 and 0.131 for both fuels.  $T_{\max}$  and  $T_{\text{avg}}$  are the maximum and the average combustor exit gas temperatures respectively;  $T_{\text{inlet}}$  is the combustor air inlet temperature. The combustor gas temperature profiles and the combustor percent pressure loss (less than 6%) are also similar for the test and the baseline fuels for comparable operating conditions. The static pressure loss characteristics of the combustor for both fuels are shown in Figure 4-1. Figure 4-2 shows the relationship between the combustor fuel/air ratio and the gas temperature rise (i.e. combustor load). The curves with, and without water injection, are plotted.

The combustor operation on the ITSL fuel with water injection was stable and comparable to that on the baseline No. 2 fuel oil at greater than 50% load. At 30% load and a water-to-fuel ratio of 1, the burner became unstable from the quenching action of the injected water. This observed characteristic would not preclude the ITSL fuel as an acceptable fuel. The combustion turbine in utility operation would seldom, if ever, be dispatched to operate at 30% load. If it were to operate at 30%, a high water injection rate would not be required to limit the  $\text{NO}_x$  to acceptable EPA limits.

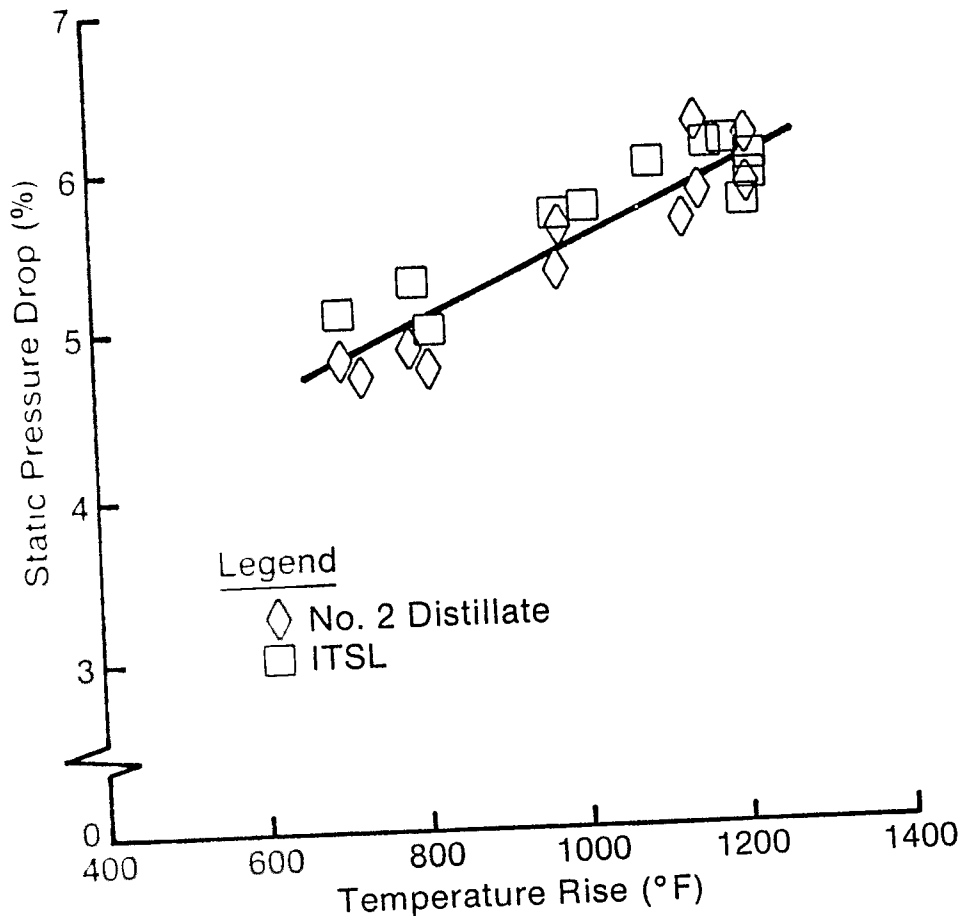


Figure 4-1. Static Pressure Drop vs. Combustor Temperature Rise



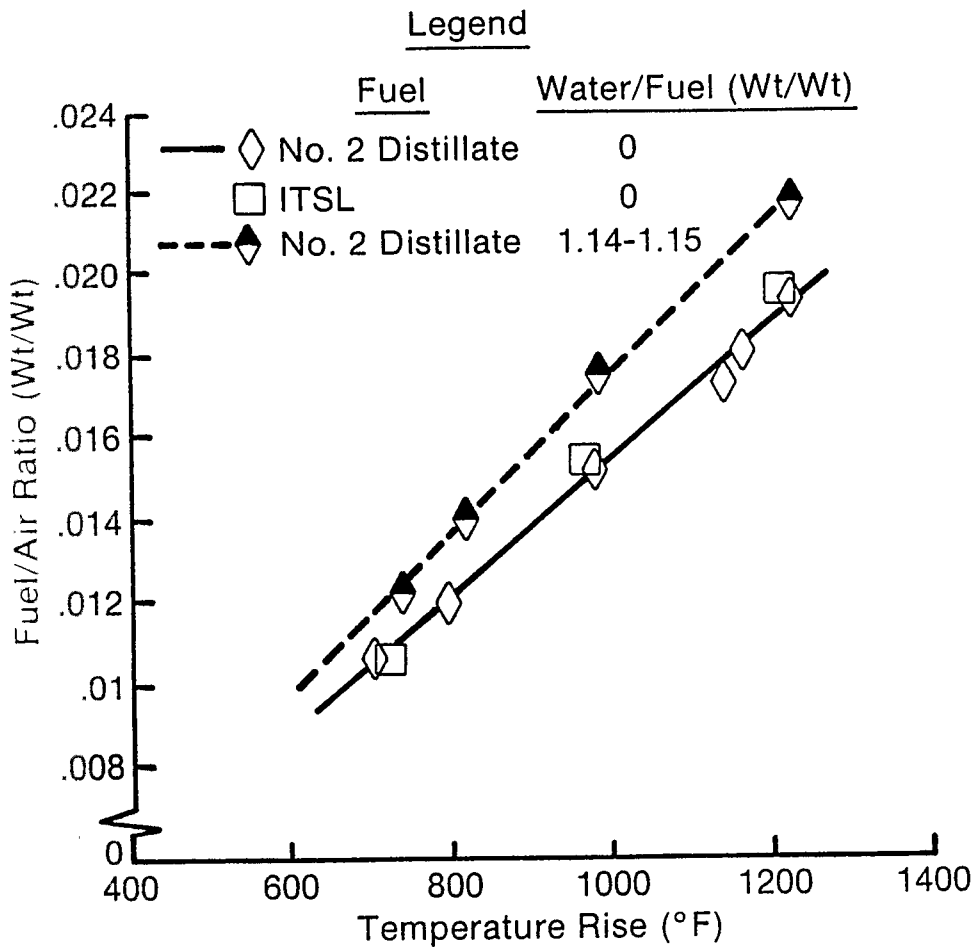


Figure 4-2. Fuel/Air Ratio vs. Combustor Temperature Rise

### Combustor Wall Metal Temperature Evaluation and Comparison with Prior Data

The combustor wall temperatures were recorded at all laboratory test conditions for the baseline No. 2 and the ITSL test fuels. The wall thermocouples used to measure local metal temperatures were located at the same positions as those on the W251AA test combustor used during the RP2112-5 engine testing of CDL fuels(1). The majority of the T/Cs were positioned on the wall of the combustor primary combustion zone (see Figure 2-2), as this is the region most affected by the flame characteristics of the fuels. The primary combustion zone contains the highest flame temperatures and the greatest flame luminosity; both factors contribute to higher thermal radiation heat loads on the combustor wall. This increased heat load results in higher wall temperatures.

Evaluation and comparison of the ITSL and baseline No. 2 test data, both with and without water injection, show the increase in wall temperatures to be consistent with expectations. Figures 4-3 through 4-5 present the wall temperature test data without water injection. The maximum metal temperature of 1506°F on combustor ring 4 when burning ITSL CDL test fuel (Figure 4-3) compared with 1402°F on No. 2 fuel (Figure 4-4) when operating at the equivalent of 100% W251AA engine base load. When the measured temperature difference was referred to the No. 2 fuel baseline load operation, a referred temperature increase of 121°F was calculated at ring 4 (Figure 4-5) where the maximum wall temperatures occur (Figures 4-3 and 4-4). The peak of the metal temperature increase from the additional flame radiant heat load, however, occurred upstream of ring 4. The referred temperature increase (above baseline No. 2 fuel oil data) of 163°F and 215°F occurred at combustor ring 2 at the 100% and 75% load condition respectively (see Figure 4-5). In the primary combustion zone the wall temperature increase ranged from about 75°F to 215°F over the test load range. The downstream air dilution zone showed increases in temperature of about 25°F, or less.

Figures 4-6 and 4-7 show the effect of water injection on wall temperatures. The water injection effect overshadows the increased flame radiation effect in the primary zone of the combustor. The net effect of water injection on the combustor wall temperatures was a major reduction in temperature level in the primary combustion zone region. The effect in the downstream air dilution region was much less pronounced as is shown in the figures.

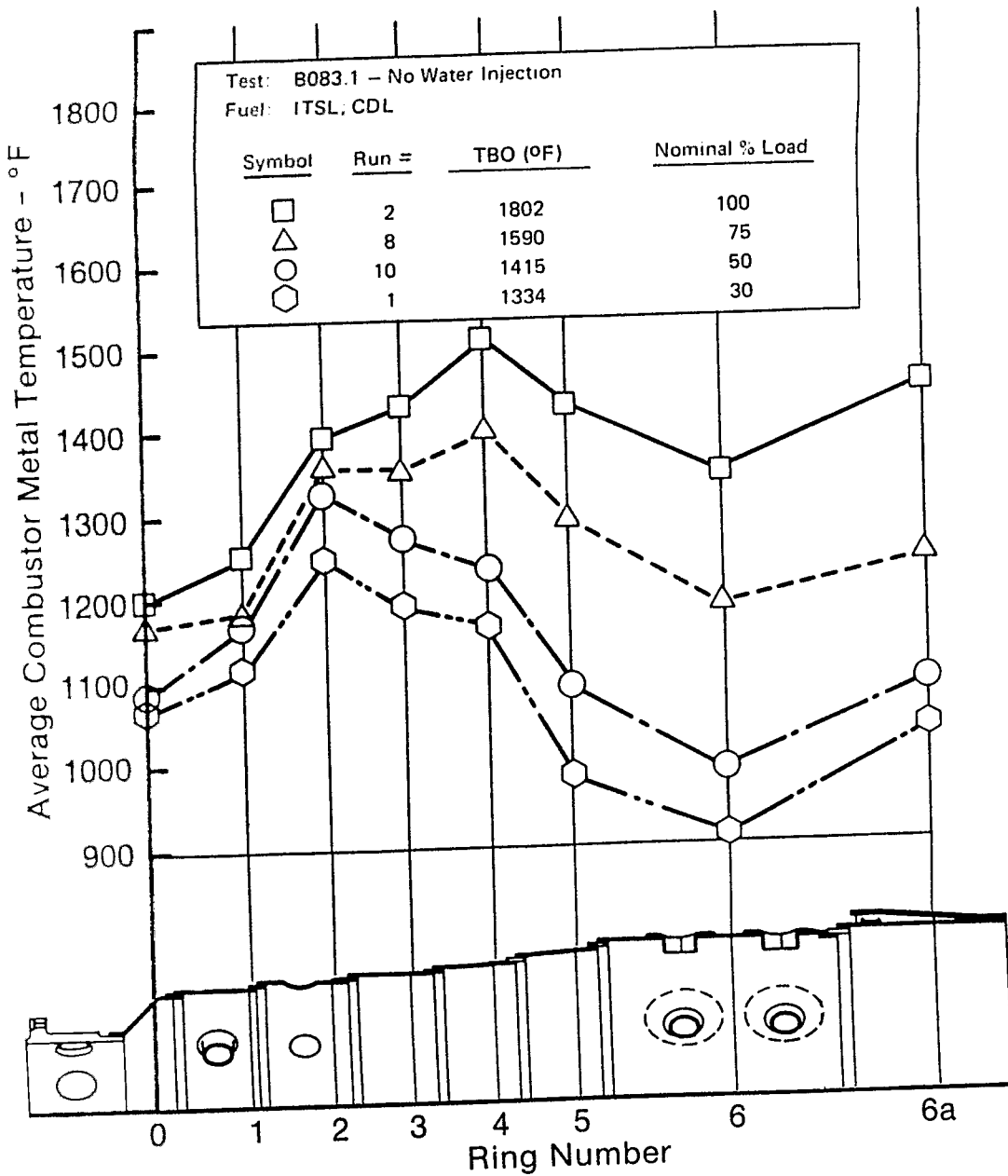


Figure 4-3. Average Combustor Metal Temperature vs. Ring Number (ITSL CDL Fuel)

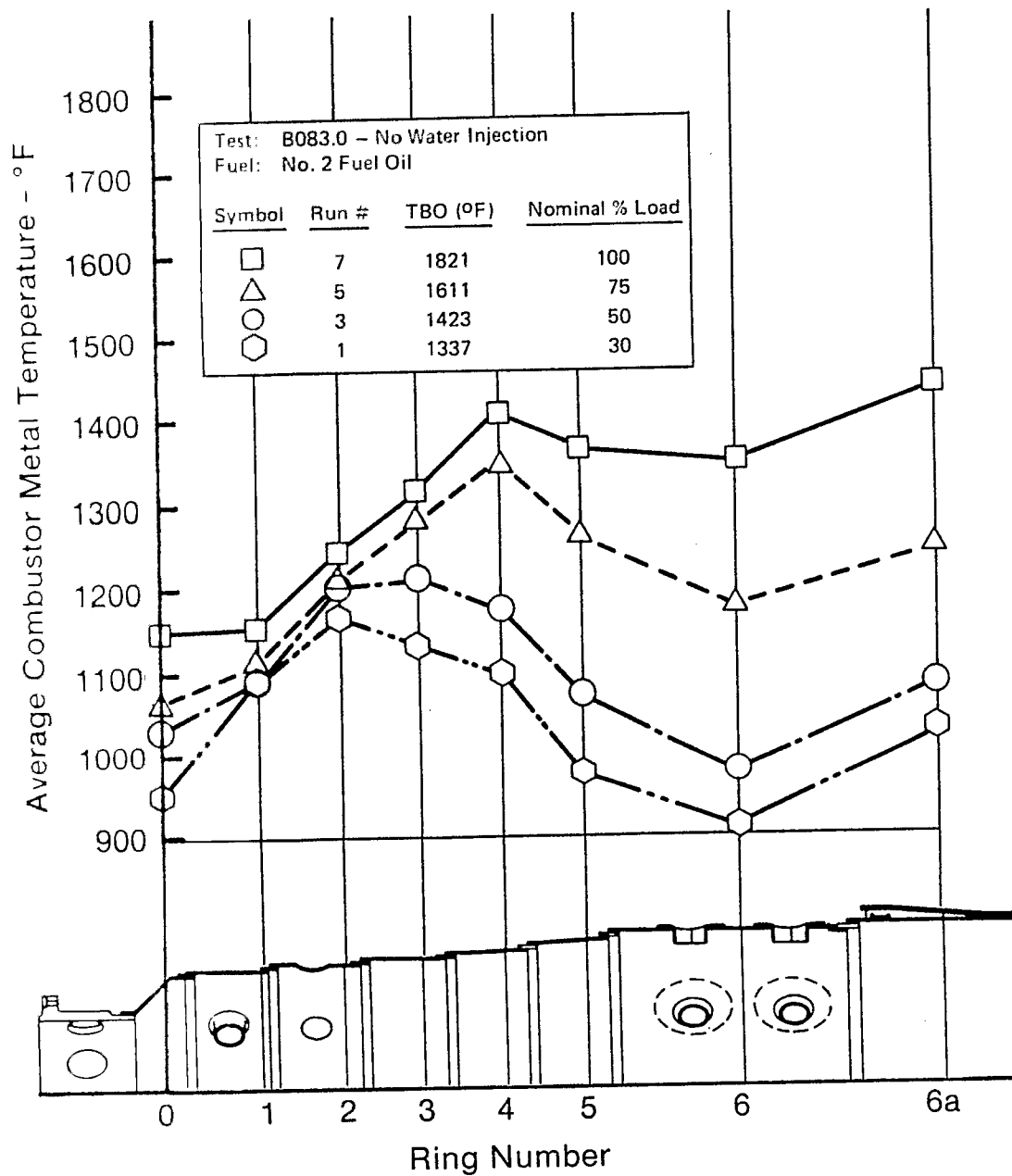


Figure 4-4. Average Combustor Metal Temperature vs. Ring Number (Baseline No. 2 Fuel Oil)

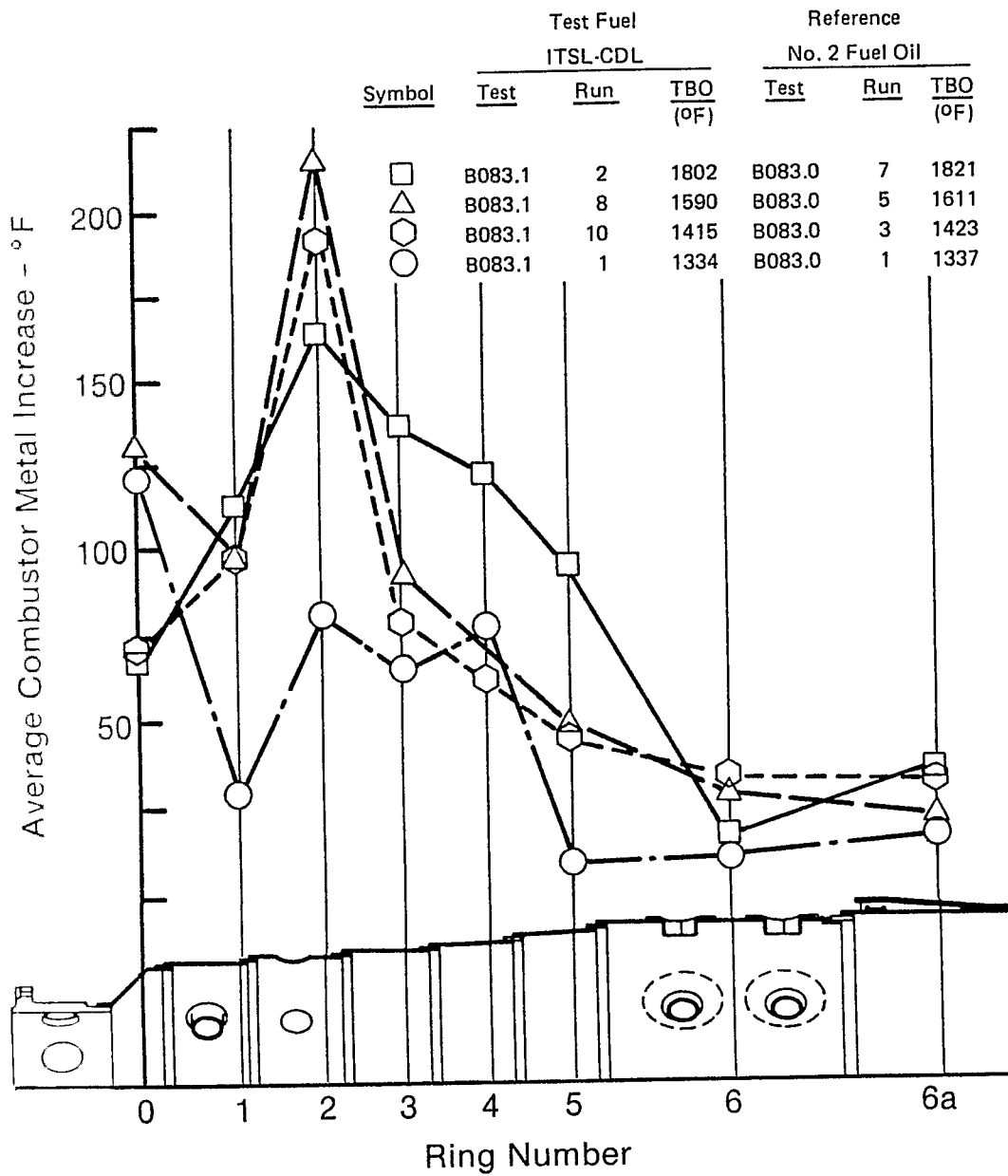


Figure 4-5. Combustor Metal Temperature Increase with ITSL Fuel

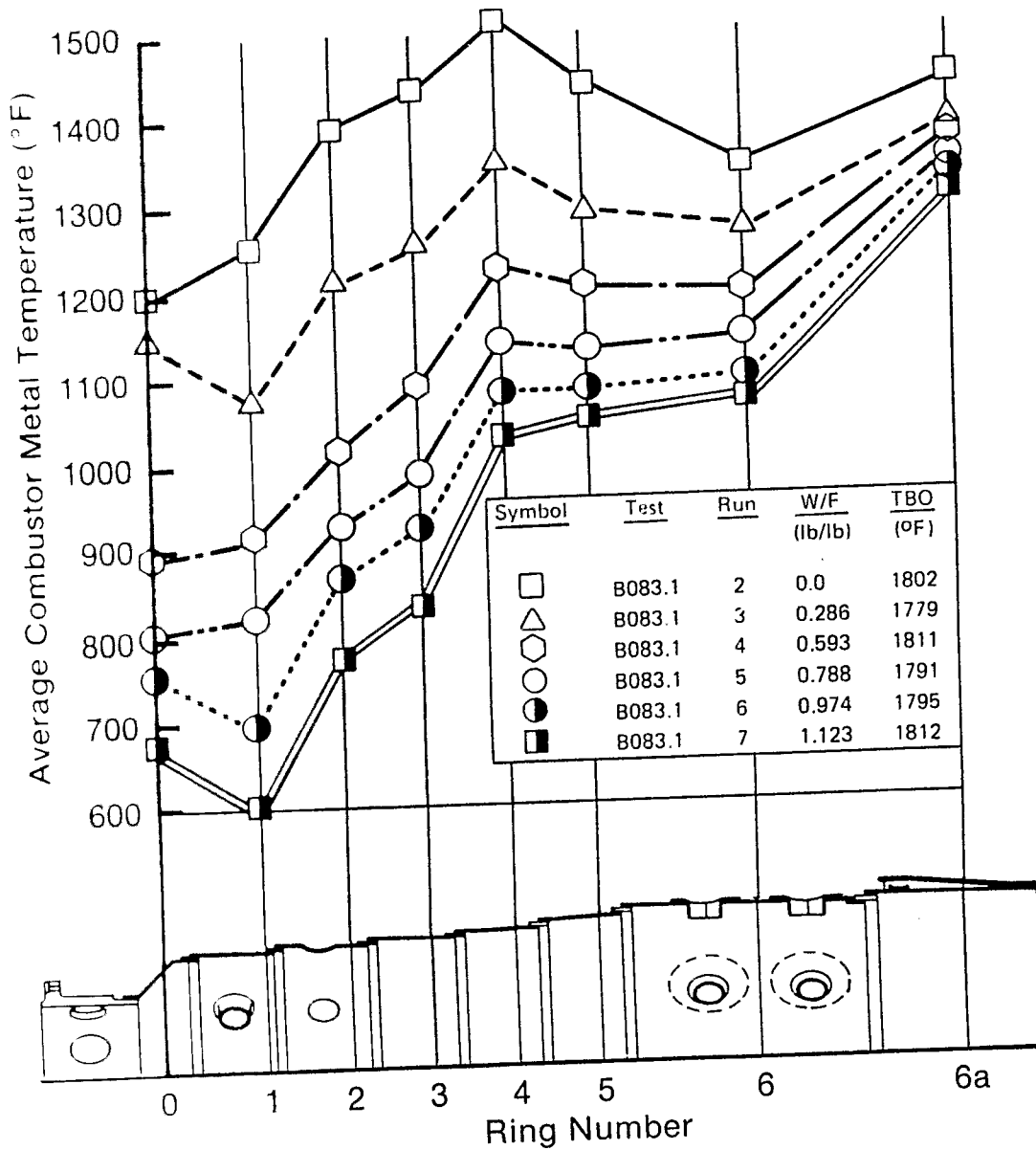


Figure 4-6. Effect of Water Injection on Metal Temperatures (at 100% Load and Burning ITSL Fuel)

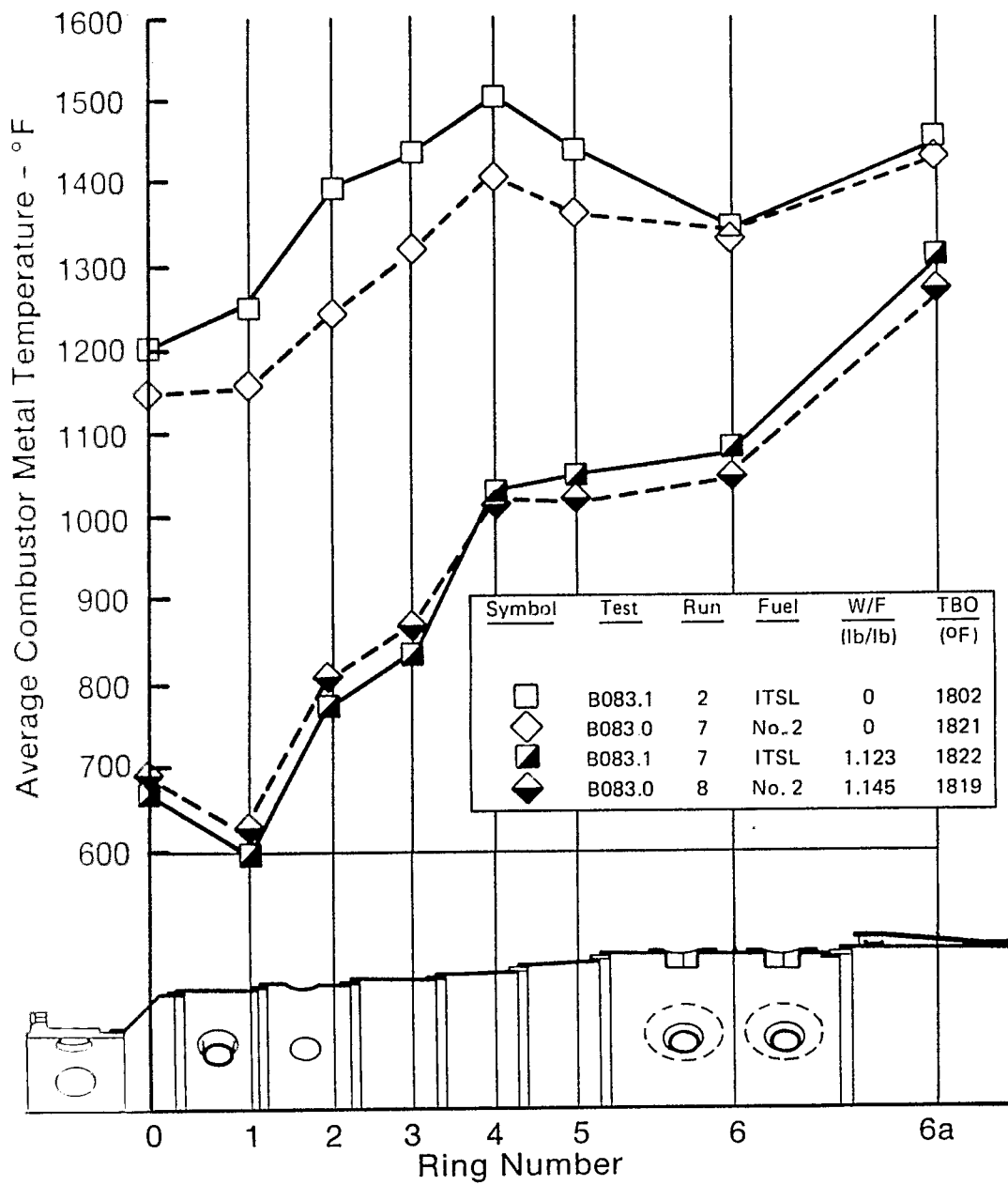


Figure 4-7. Comparison of Metal Temperatures With and Without Water Injection (at 100% Load)

Comparison of the ITSL test data with the prior data base developed during the engine testing of H-Coal and EDS CDL fuels(1), and earlier data from the EPRI RP989-1 test program(2), is presented in Figures 4-8 through 4-14. Figures 4-8 through 4-12 present wall temperature data compared in various ways. Figures 4-8 and 4-9 show the data vs. ring location for the CDL fuels and the baseline No. 2 fuel oil respectively. Figure 4-10 depicts the temperature increase (above baseline No. 2 fuel oil data) for the CDL fuel operation. Figure 11 presents the effect of water injection on the rings with highest metal temperatures. Similarity of the ITSL fuel laboratory and the EDS field test data is apparent. Figure 4-12 presents the maximum wall temperature increase (at maximum burner outlet temperature) for the ITSL fuel plotted on field test data curve reported in Reference (1). Reasonable agreement is seen.

A correlation of the wall temperature data base was made using a dimensionless temperature parameter,  $TP(R)$ , that referred the CDL wall temperature data to the baseline No. 2 fuel load conditions so that the evaluation of data could be made using a common base for comparison. With the exception of the PECO H-Coal data, the referred temperature parameter,  $TP(R)$ , correlated well as a linear function of the hydrogen content ( $\%H_2$  by weight) (see Figure 4-13). The correlation factor,  $r$ , for all CDL data (excepting the field H-Coal data) is above  $-0.90$  for all rings. Values of  $r$  above  $-0.90$  show a very high degree of correlation. A ring-by-ring correlation of  $TP(R)$  was also made against the fuel carbon-to-hydrogen ratio (C/H) by weight (see Figure 4-14). This correlation also had very high correlation coefficients, generally above  $+0.90$ . The H-Coal wall temperatures did not correlate with other data during the analysis of the PECO test data. This deviation from expected was attributed, at that time, to the high iron content (28 ppmw) of the H-Coal(1). Iron compounds are sometimes used as smoke reduction additives. This would affect the flame radiation characteristics.

The data correlations provide information that can be used by the hardware designer to determine whether low hydrogen fuels, such as is typical of coal-derived fuels, are acceptable for use with conventionally film cooled combustors similar to the test combustor used for the fuels evaluation, or whether hardware design changes to improve wall cooling would be necessary. The laboratory test data on the ITSL CDL test fuel show that, although the wall temperatures do increase because of the more highly radiant flame, the fuel is an acceptable combustion turbine fuel. However, the combustor wall cooling needs must be satisfied to maintain wall temperatures within defined limits to provide the required long life operation.



Symbol	Test	Run	CDL Fuel	TBO (°F)	H <sub>2</sub> Content % by Wt
□	RP2112-5 - Lab	2	ITSL-CDL	1821	10.91
▽	RP2112-5 - Field	2.6	H-Coal	1764	10.48
▼	RP2112-5 - Field	3.6	EDS	1836	10.16
△	RP989 - Lab	388	H-Coal (≠2)	1851	11.48
◇	RP989 - Lab	415	SRCII Blend	1939	8.70

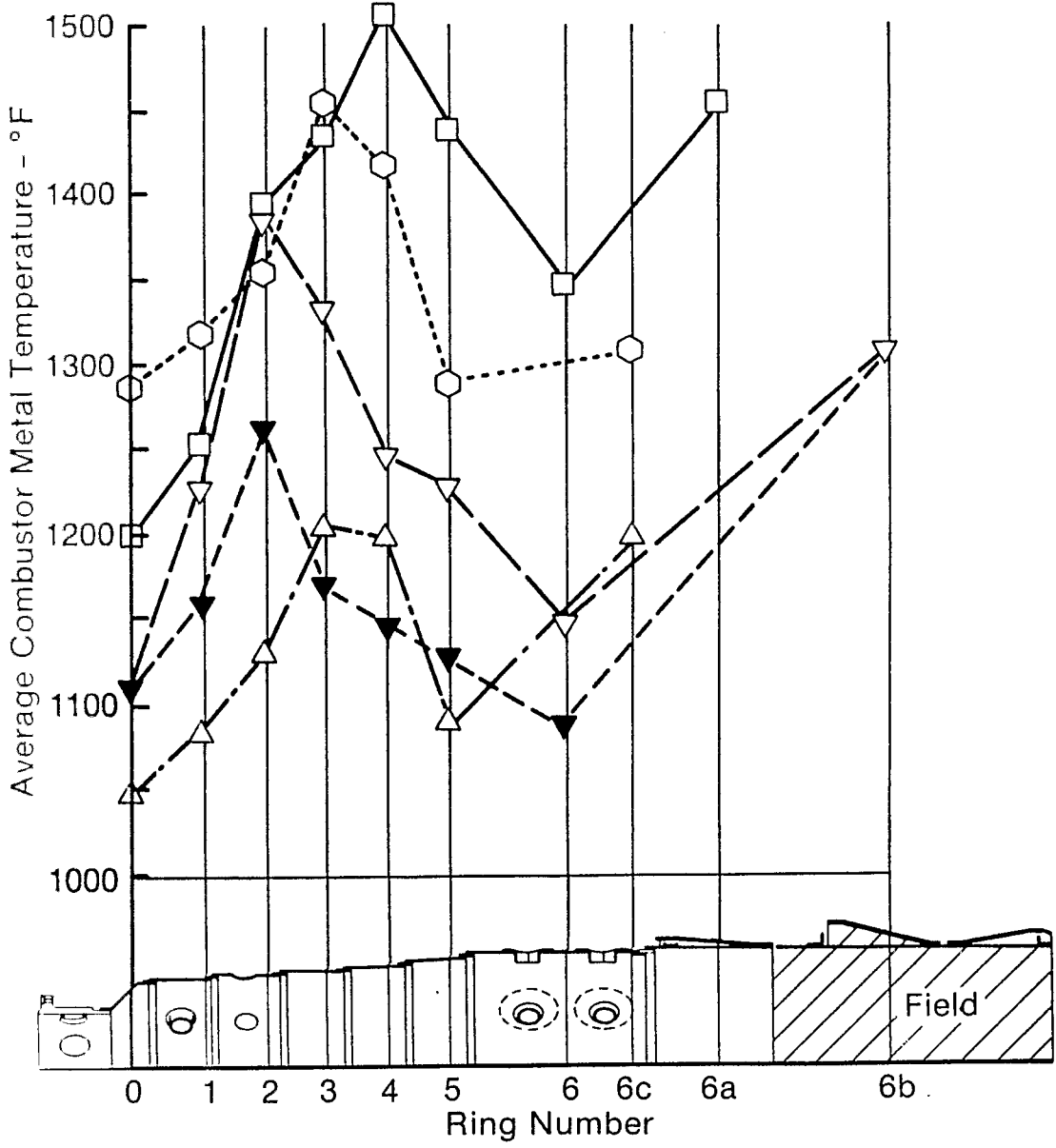


Figure 4-8. Comparison of Combustor Metal Temperatures Burning ITSL Fuel With Field and RP 989-1 CDL Data Base (At Maximum Burner Outlet Temperature)

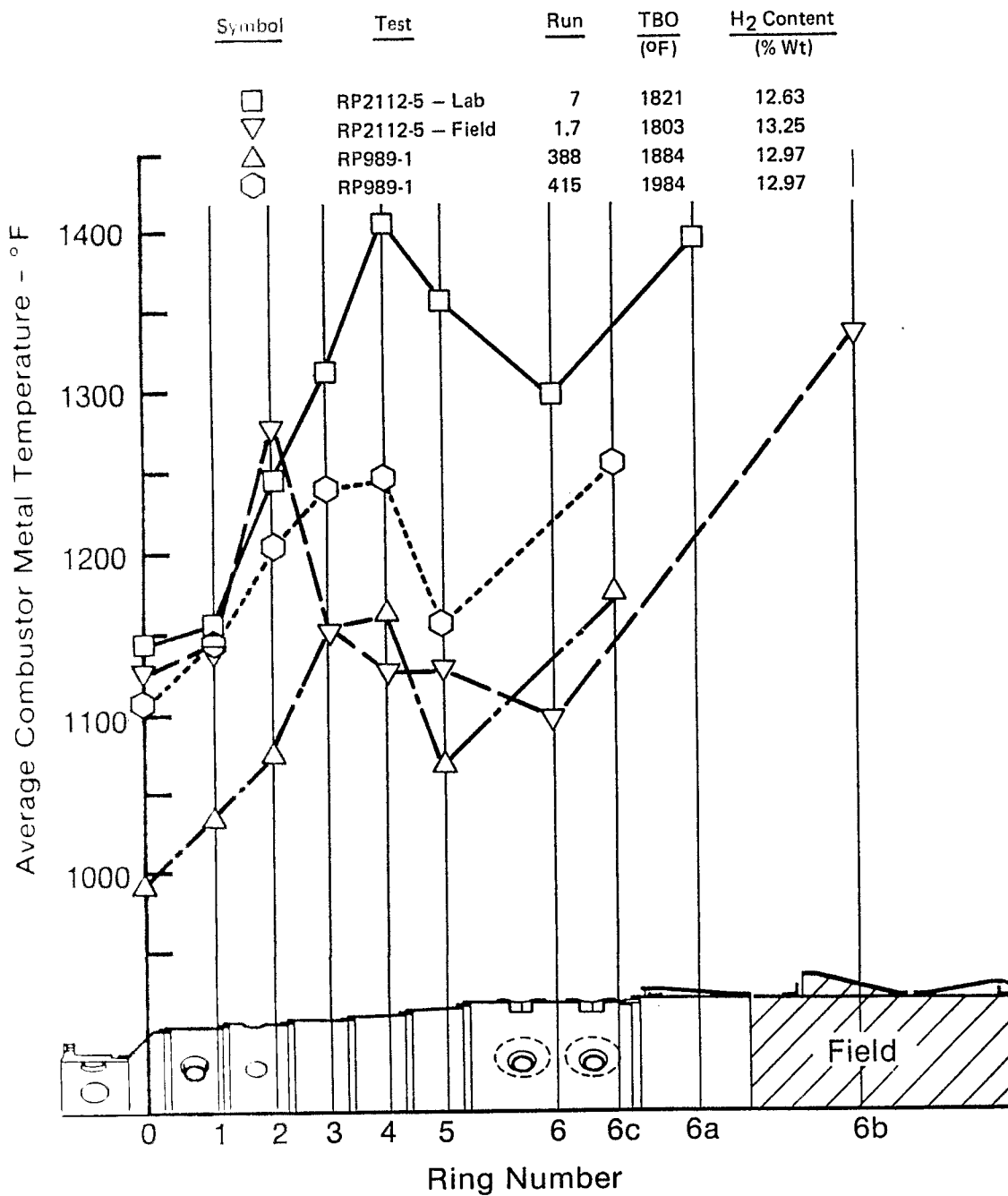


Figure 4-9. Comparison of Laboratory and Field Combustor Metal Temperatures Burning Baseline No. 2 Fuel Oil (At Maximum Burner Outlet Temperature)

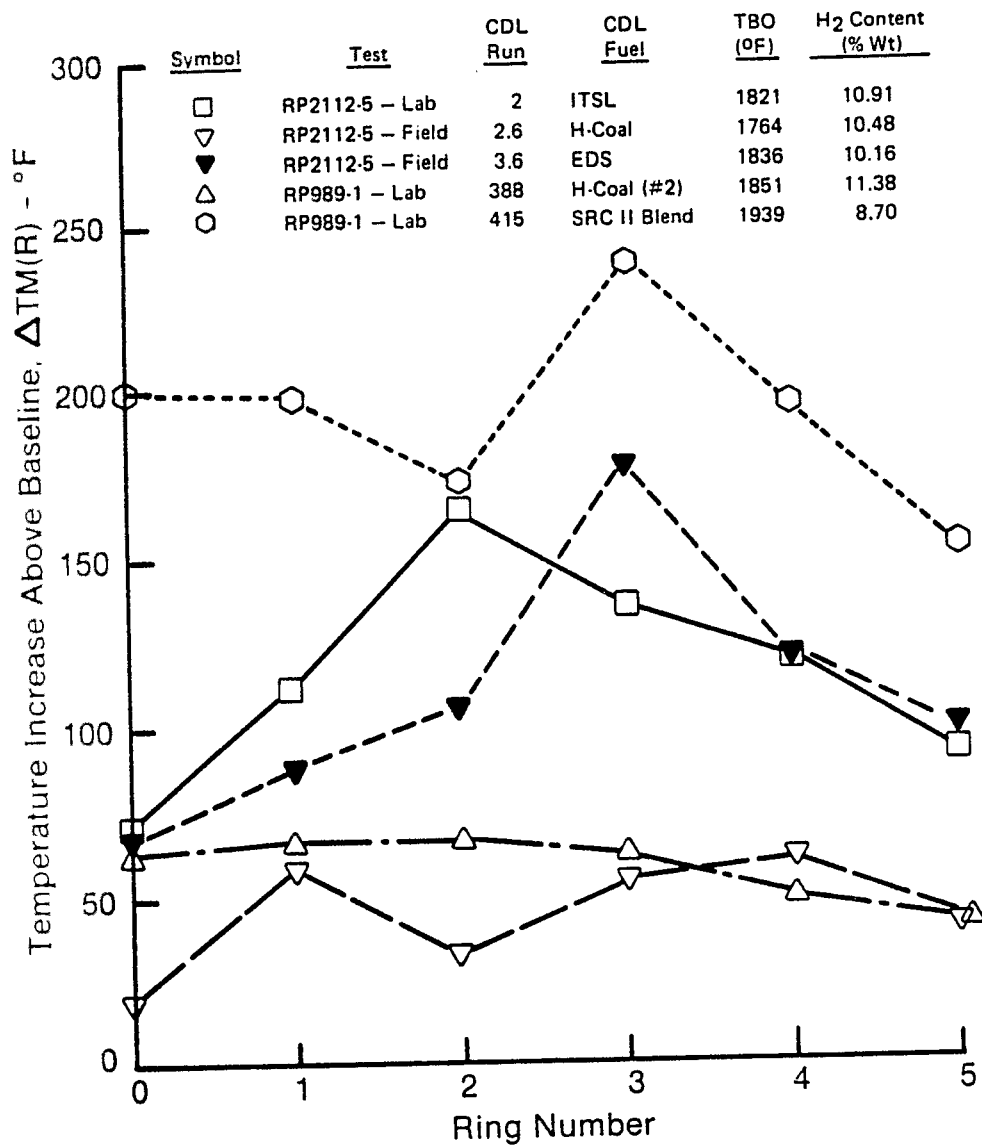


Figure 4-10. Combustor Metal Temperature Increase for CDL Fuels (Field and Laboratory Tests at 100% Load)

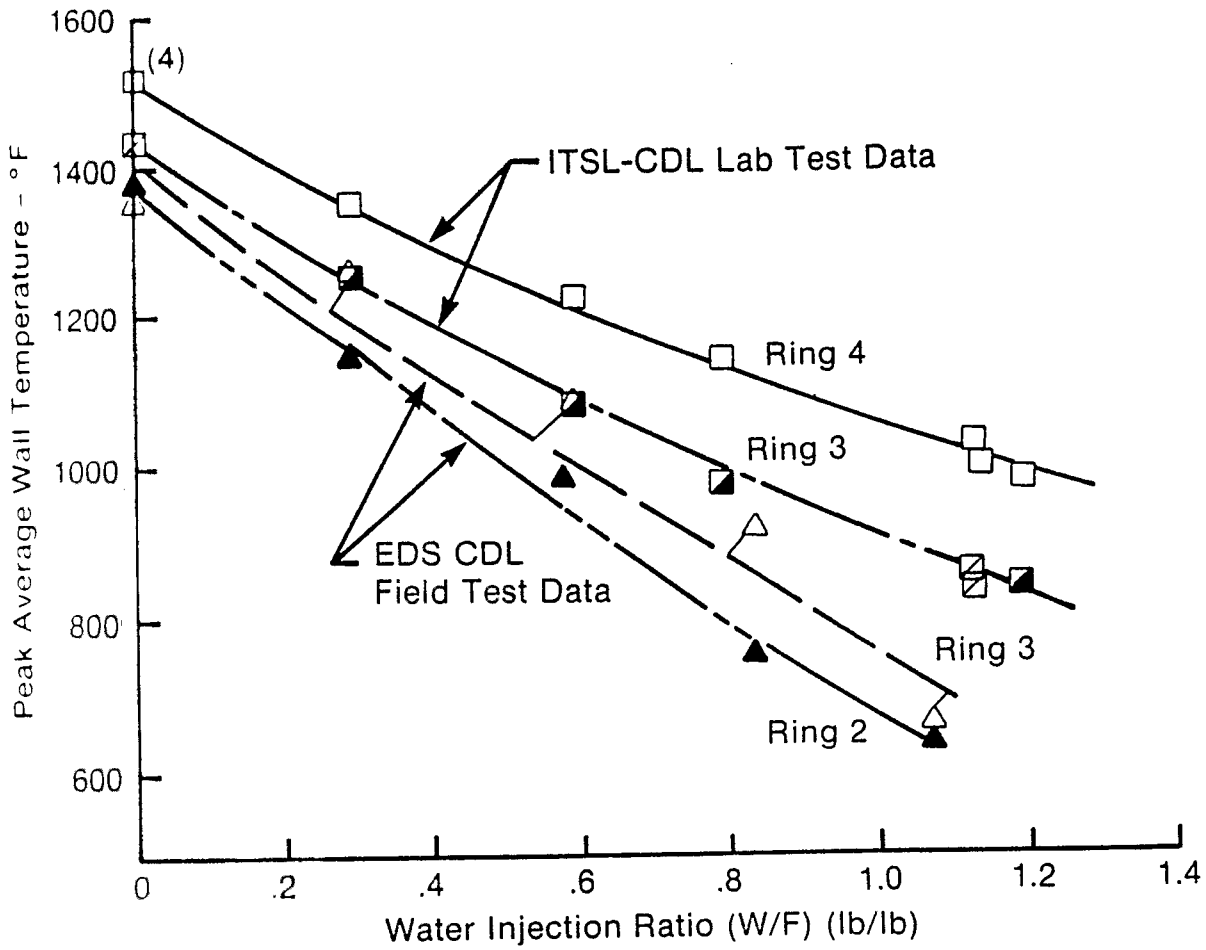


Figure 4-11. Water Injection Effect on Average Metal Temperatures (Field and Laboratory Tests at 100% Load)

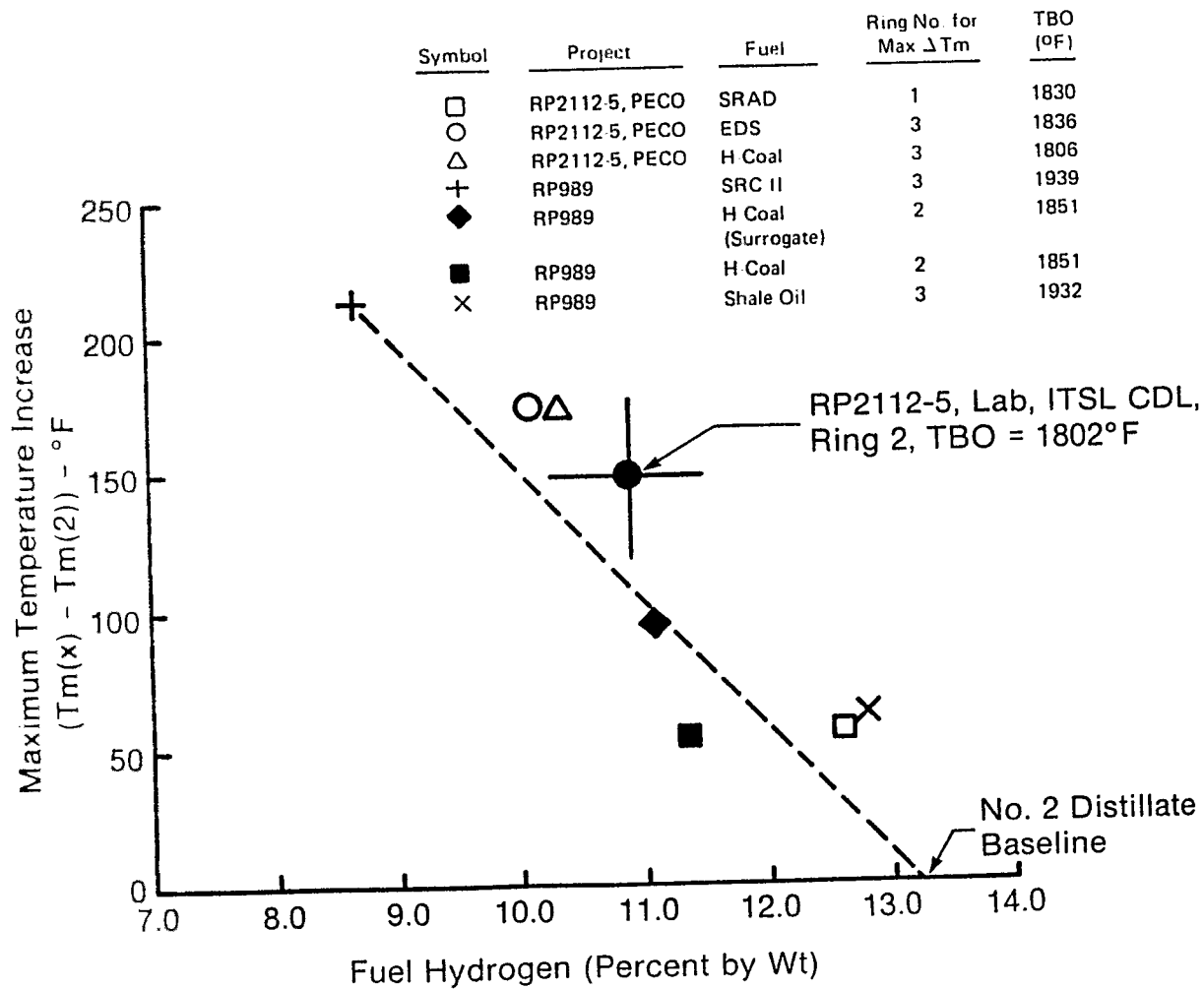


Figure 4-12. Comparison of Maximum Temperature Increase vs. Hydrogen Content (Field and Laboratory Tests at Maximum Burner Outlet Temperature)

$$TP(R) = \frac{[TM(x) - TC(x)] \times LP - [TM(2) - TC(2)]}{[TM(2) - TC(2)]}$$

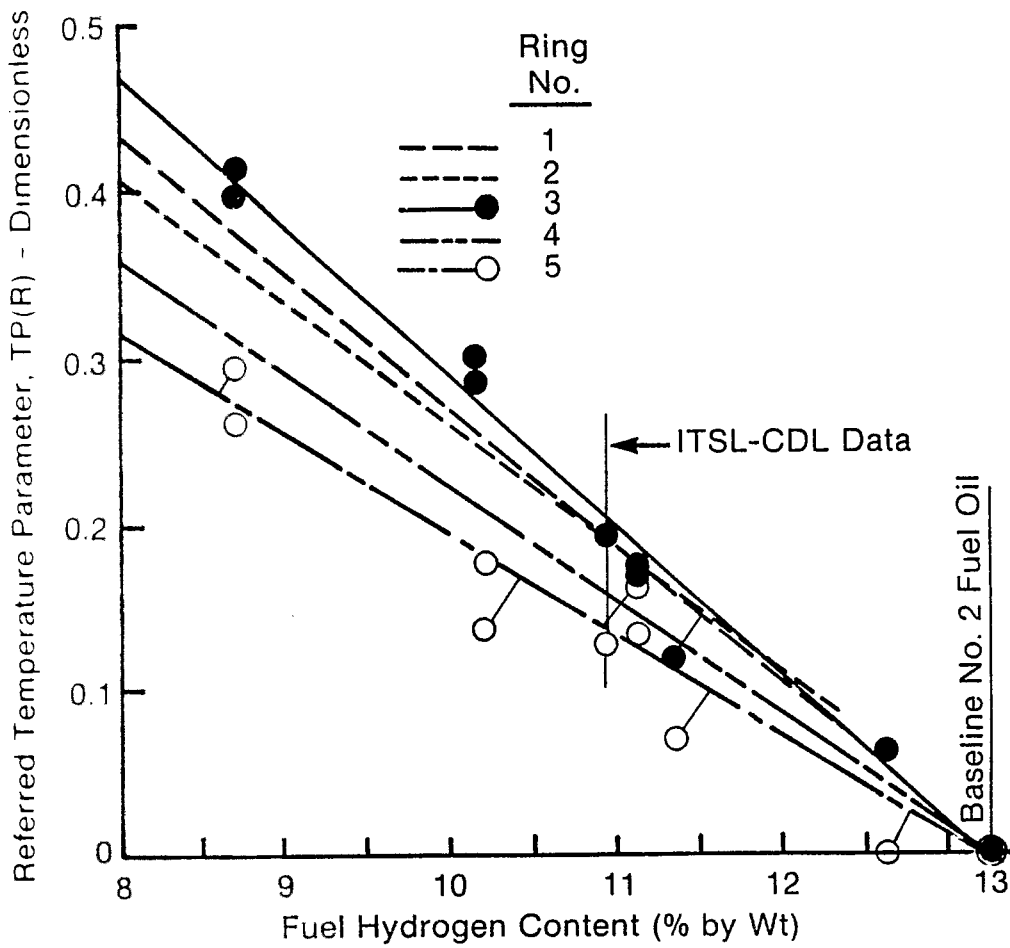


Figure 4-13. Referred Temperature Parameter vs. Hydrogen Content (For 100% Load Test Conditions)

$$TP(R) = \frac{[TM(x) - TC(x)] \times LP - [TM(2) - TC(2)]}{[TM(2) - TC(2)]}$$

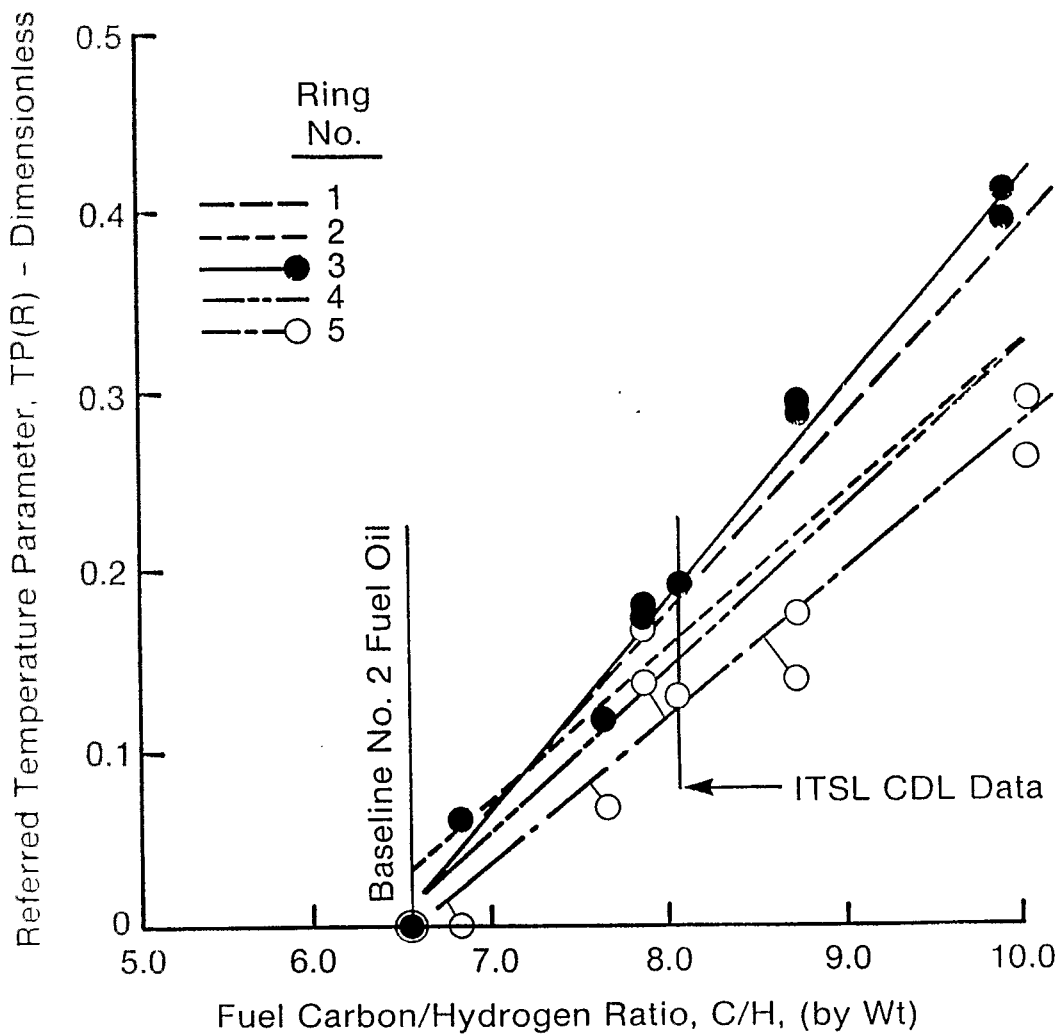


Figure 4-14. Referred Temperature Parameter vs. Fuel Carbon/Hydrogen Ratio (For 100% Load Test Conditions)

The ITSL test data complement and extend the CDL data base for evaluation of coal-derived liquid fuels. From the standpoint of comparing and correlating the laboratory wall temperature data with previous test results, the objectives of the experimental program were achieved.

#### Emissions Test Results and Comparison with Prior Data

Emissions were measured for the two combustion test series (ITSL CDL and No. 2 fuels) over an equivalent load range of 30% to 100% engine base load. Both test series included the effects of water injection into the burner.

The measured  $\text{NO}_x$  emissions in the products-of-combustion at the combustor exit are reported in Figure 4-15. The data normalized to EPA ISO-standard conditions of ambient temperature, pressure, and humidity, and corrected to 15% oxygen, standard engine heat rate and allowance for fuel-bound nitrogen were determined, and are shown in Figure 4-16. The expected increase in the measured  $\text{NO}_x$  emissions with increasing combustor rise (load), or outlet gas temperature, was observed. The ITSL CDL fuel measured  $\text{NO}_x$  values were about 30 ppmv (dry) above the baseline No. 2 fuel  $\text{NO}_x$  values near 100% load ( $\sim 1180^\circ\text{F}$  temperature rise). This difference is attributed primarily to the higher FBN (0.13% wt vs  $<0.01\%$ ) in the CDL fuel. Both sets of  $\text{NO}_x$  data show linear variation with increasing load within the range of data.

The EPA normalized ITSL CDL data are compared with the field data in Figure 4-17. The EPA data for the CDL fuels can be reasonably fitted with a straight lines. All CDL fuels show similar characteristics.

The usual effect of water injection into the combustion chamber reducing the thermal  $\text{NO}_x$  generation was observed when burning the ITSL CDL and No. 2 fuels. The reduction of  $\text{NO}_x$  as a function of water-to-fuel ratio (W/F) for the ITSL laboratory test was very similar to that observed for EDS fuel during the field tests as shown in Figure 4-18. A water-to-fuel (W/F) ratio of about 0.4 reduces the EPA normalized  $\text{NO}_x$  to about 75 ppmv (dry). The field and laboratory data show that the W/F ratio required for compliance with the EPA requirement of 75 ppmv  $\text{NO}_x$  increases linearly with the fuel bound nitrogen content at the rate of 1.5 W/F ratio per FBN (%). The EPA  $\text{NO}_x$  limits can be realized with water injection.



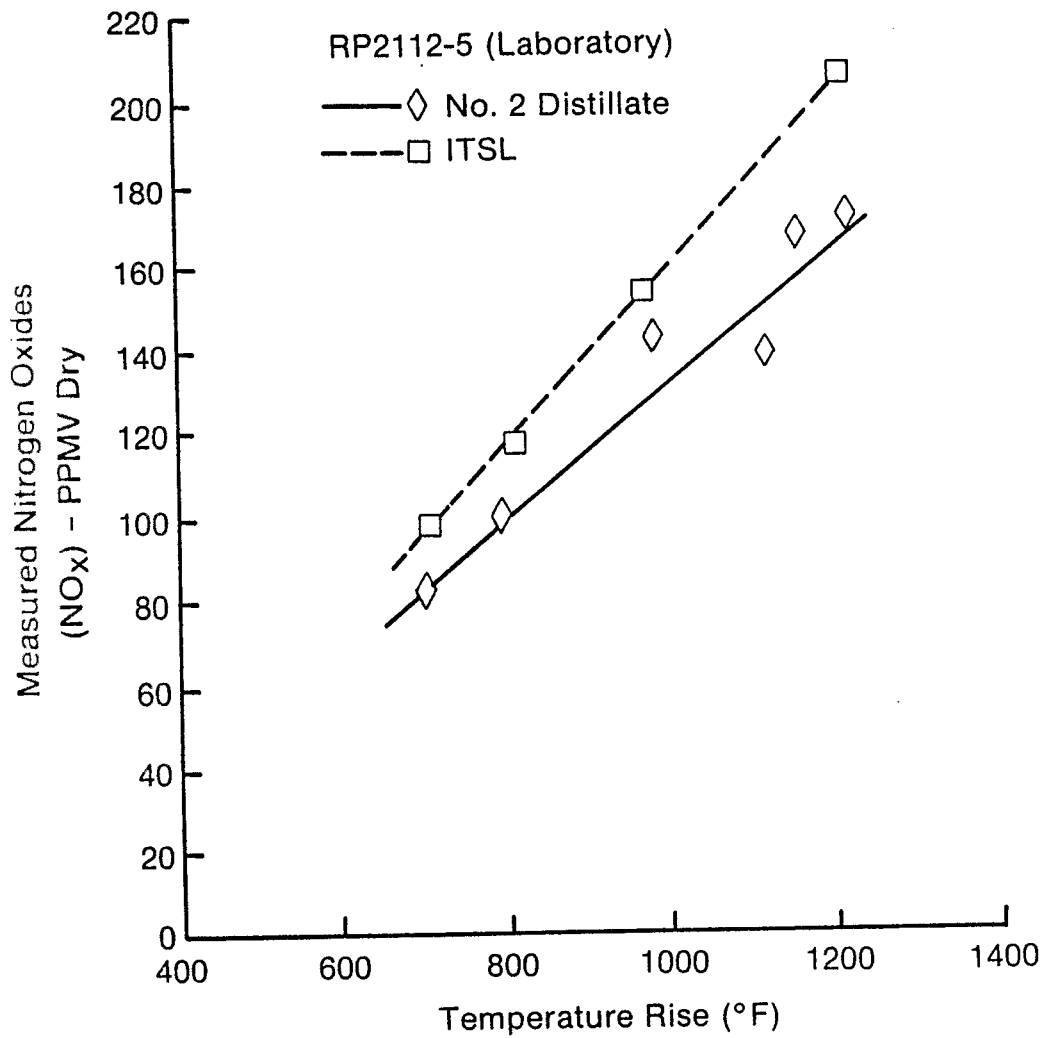


Figure 4-15. Measured Nitrogen Oxides vs. Temperature Rise

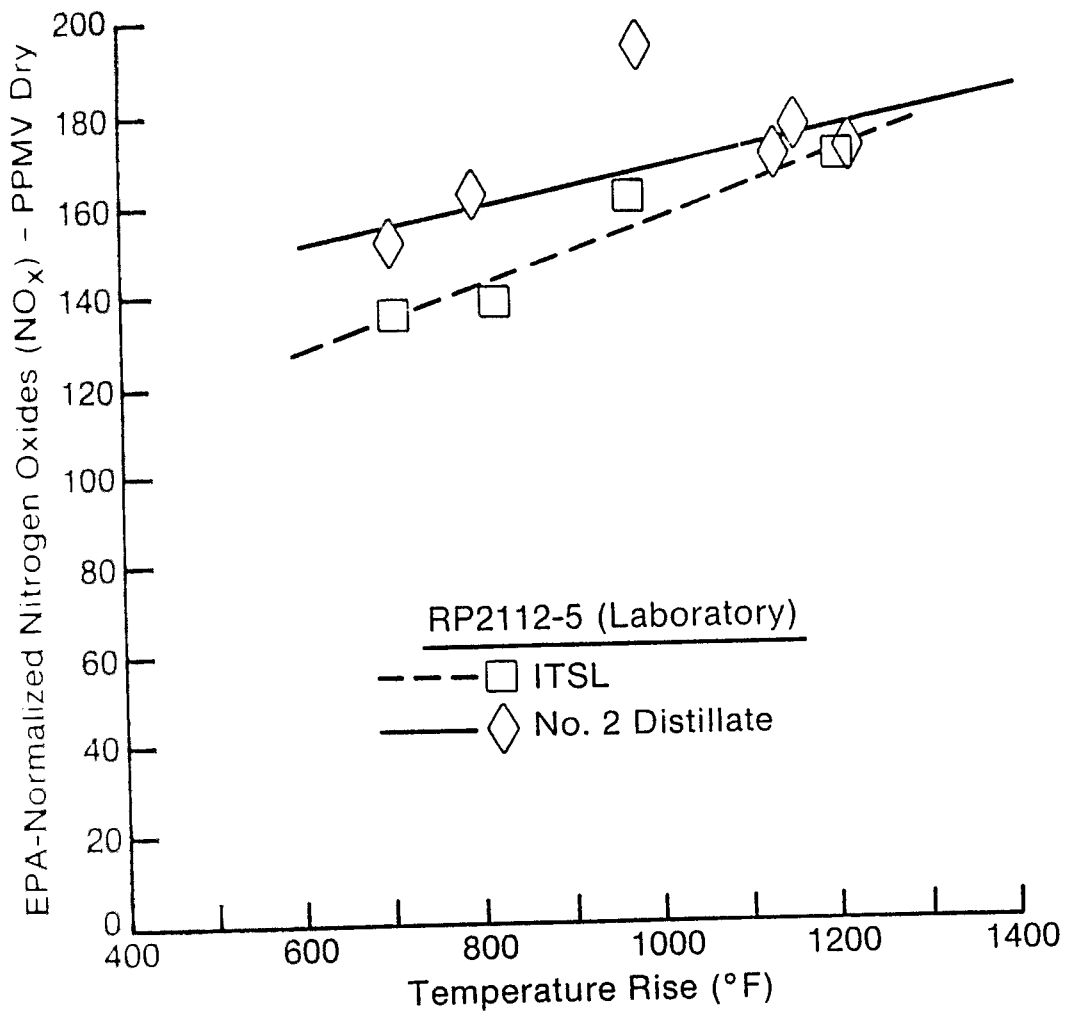


Figure 4-16. EPA-Normalized Nitrogen Oxides vs. Temperature Rise

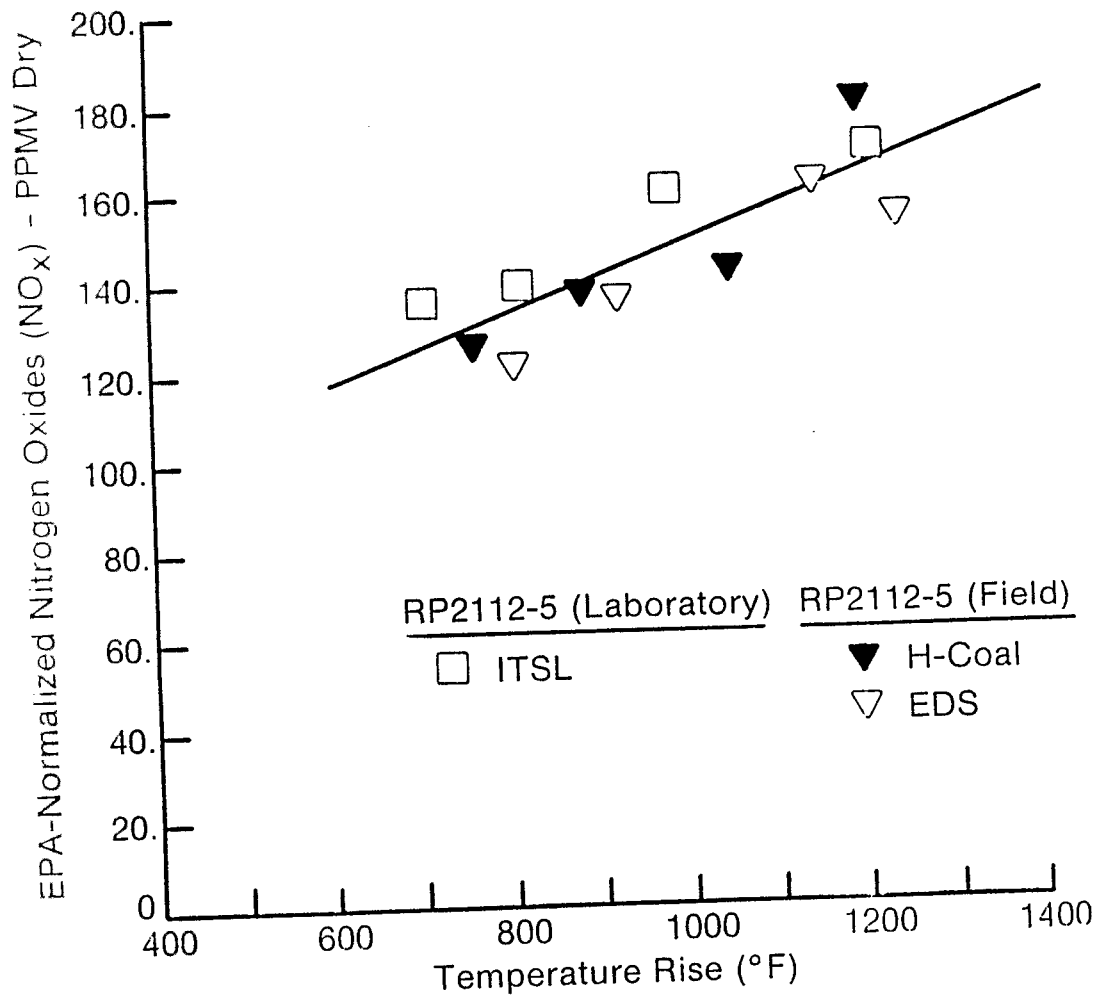


Figure 4-17. Comparison of Field and Laboratory EPA-Normalized NO<sub>x</sub>

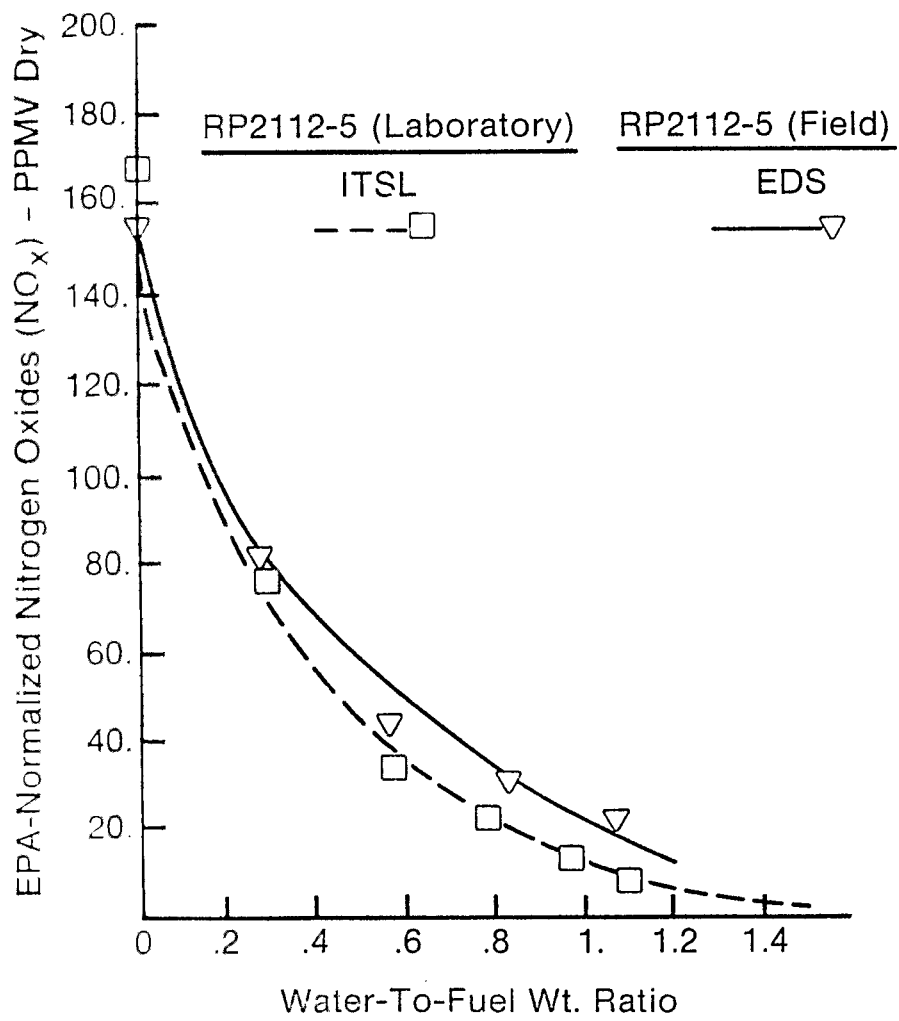


Figure 4-18. Comparison of Effect of Water Injection on NO<sub>x</sub> (Field and Laboratory)

Other emissions, such as CO, UHC, O<sub>2</sub>, and CO<sub>2</sub> for the ITSL CDL fuel generally followed the usual characteristics with load and with water injection. Figure 4-19 presents the carbon monoxide, without water injection, as a function of combustor temperature rise. The low CO concentration (30 ppmw or less over the combustor load range of 30 to 100%) implies high combustion efficiency. The effect of water injection on carbon monoxide concentration is shown in Figure 4-20. The higher levels of CO reflect a reduction in combustion efficiency of perhaps 1/2 percent.

Figure 4-21 compares the laboratory and field carbon monoxide emissions data. The No. 2 distillate, and the ITSL and EDS CDL, fuels data show good comparison. The field H-Coal data appears somewhat higher than other CDL comparable data. However, the low CO concentrations reflect high combustion efficiencies in all instances.

Figures 4-22 and 4-23 present the Bacharach smoke spot number as a function of combustor temperature rise and injected water/fuel weight ratio respectively. The reduction in smoke with water injection is typical of the W251AA combustion turbine burner operation. The values shown for the laboratory test data are of the same order as observed during the field testing(1).

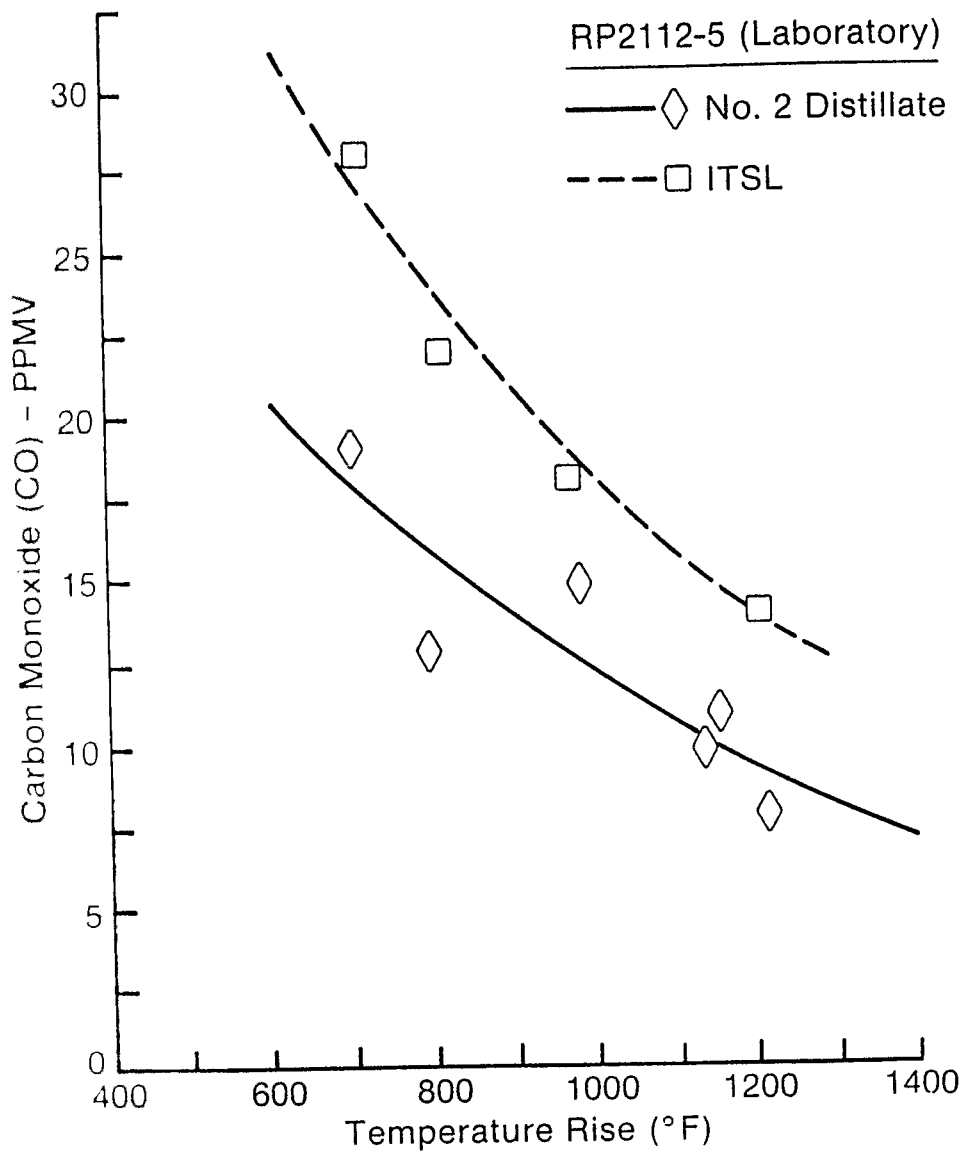


Figure 4-19. Carbon Monoxide vs. Temperature Rise (Without water Injection)

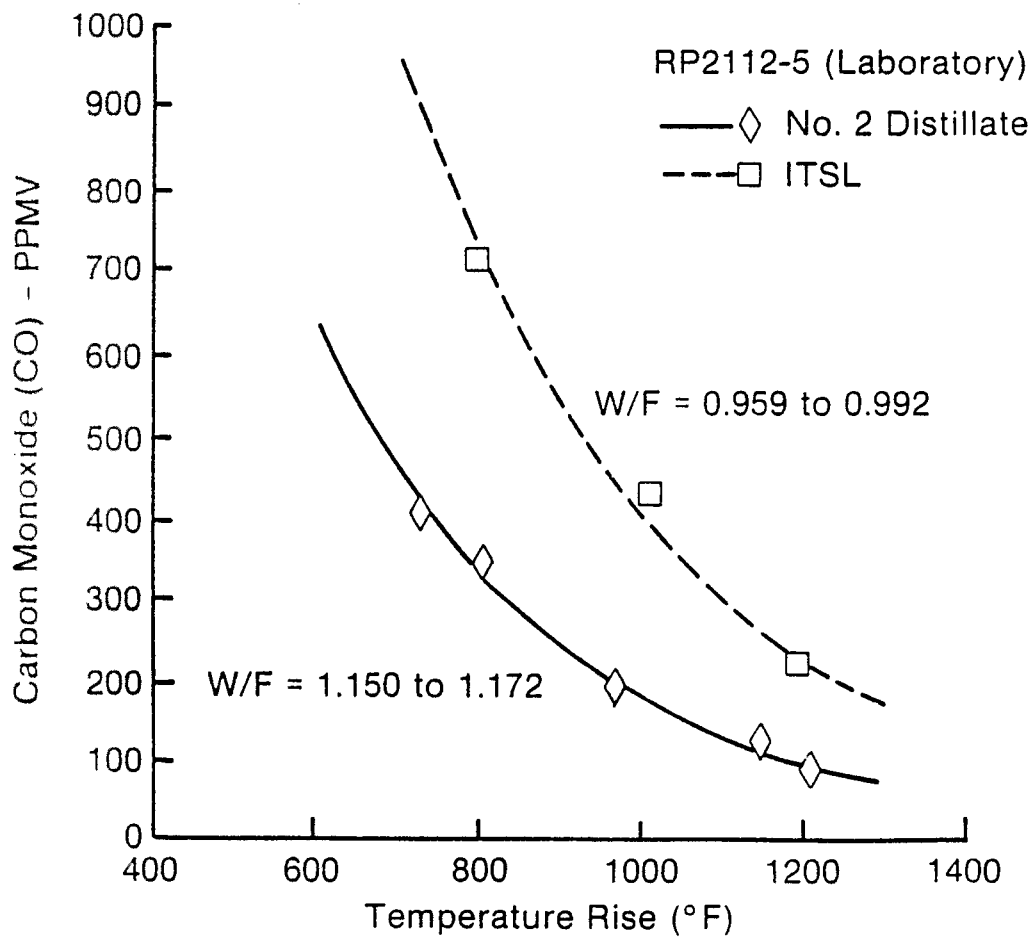


Figure 4-20. Carbon Monoxide vs. Temperature Rise  
(Water/Fuel Ratio ~1)

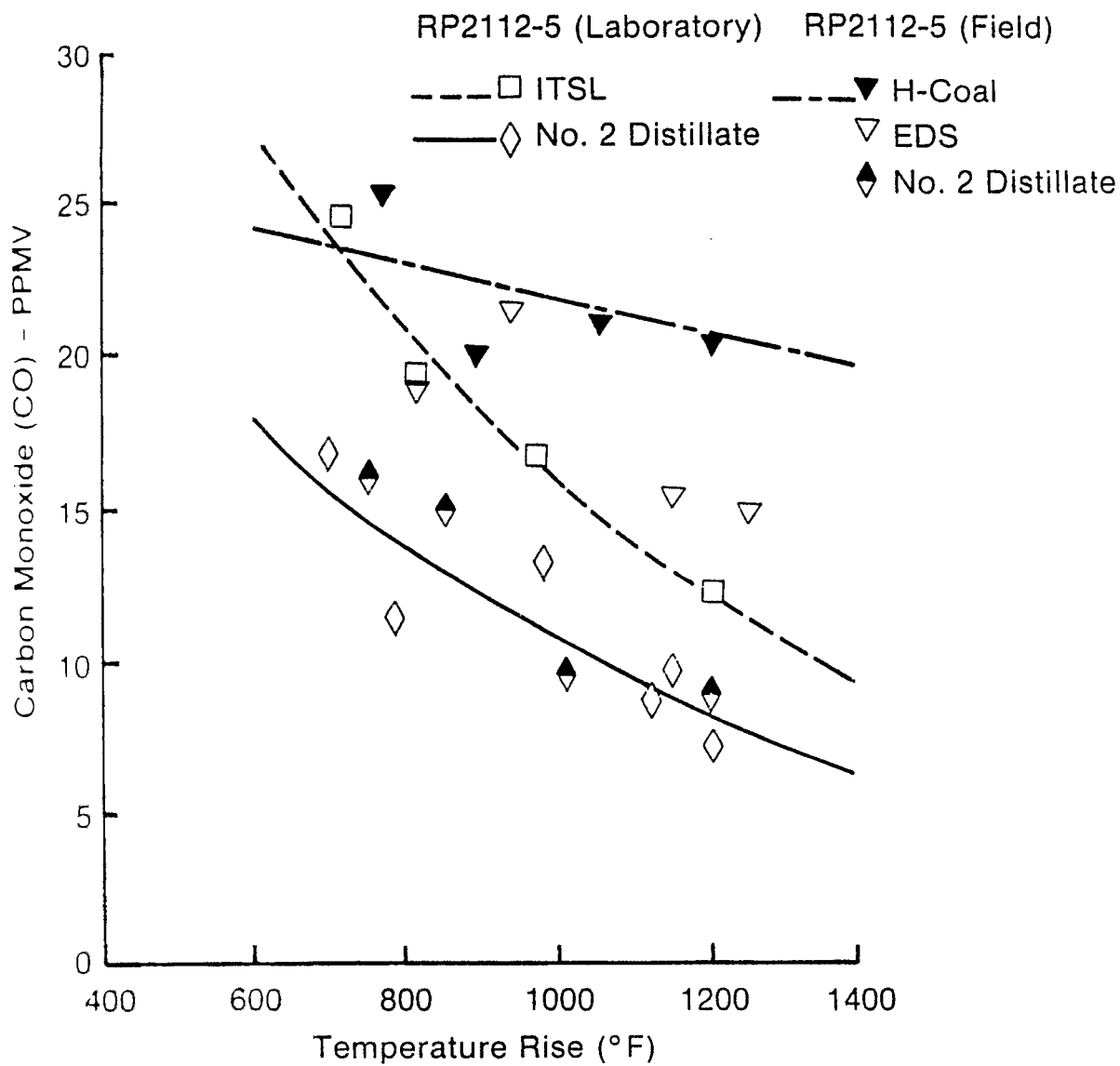


Figure 4-21. Comparison of Carbon Monoxide Emissions (Field and Laboratory)



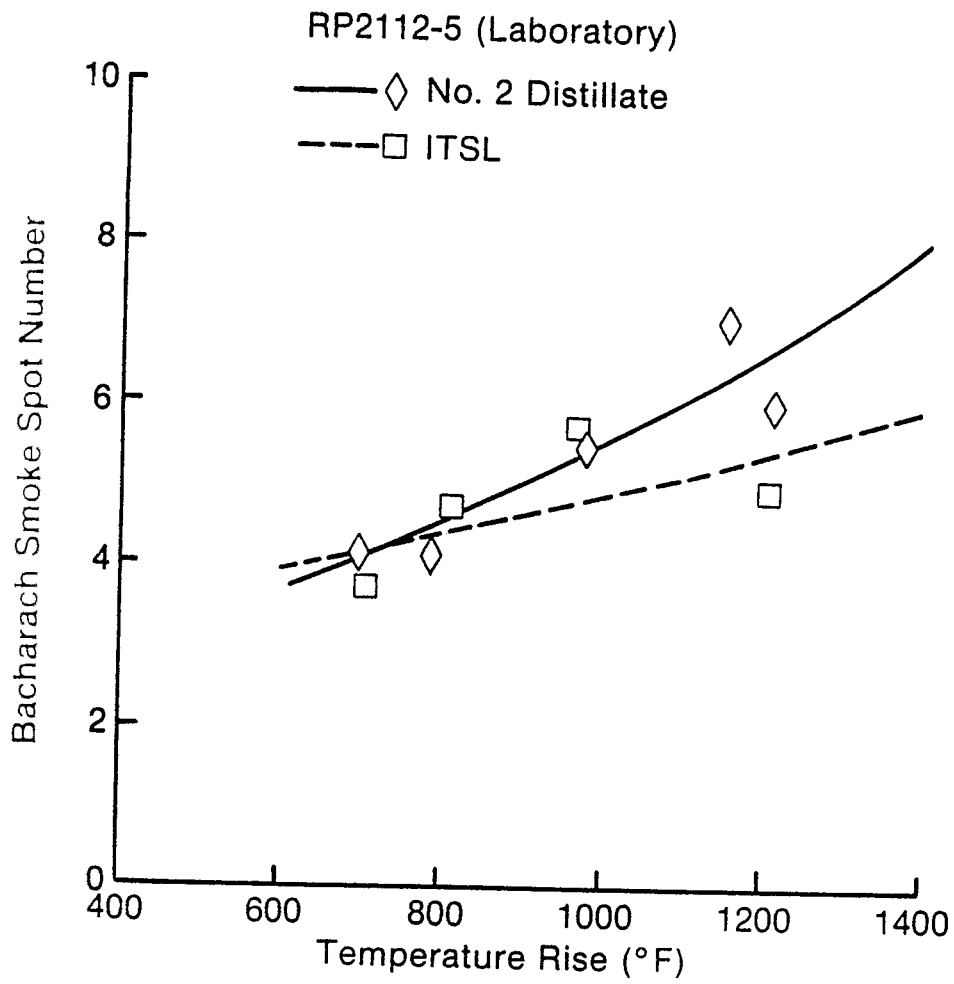


Figure 4-22. Bacharach Smoke Spot Number vs. Temperature Rise

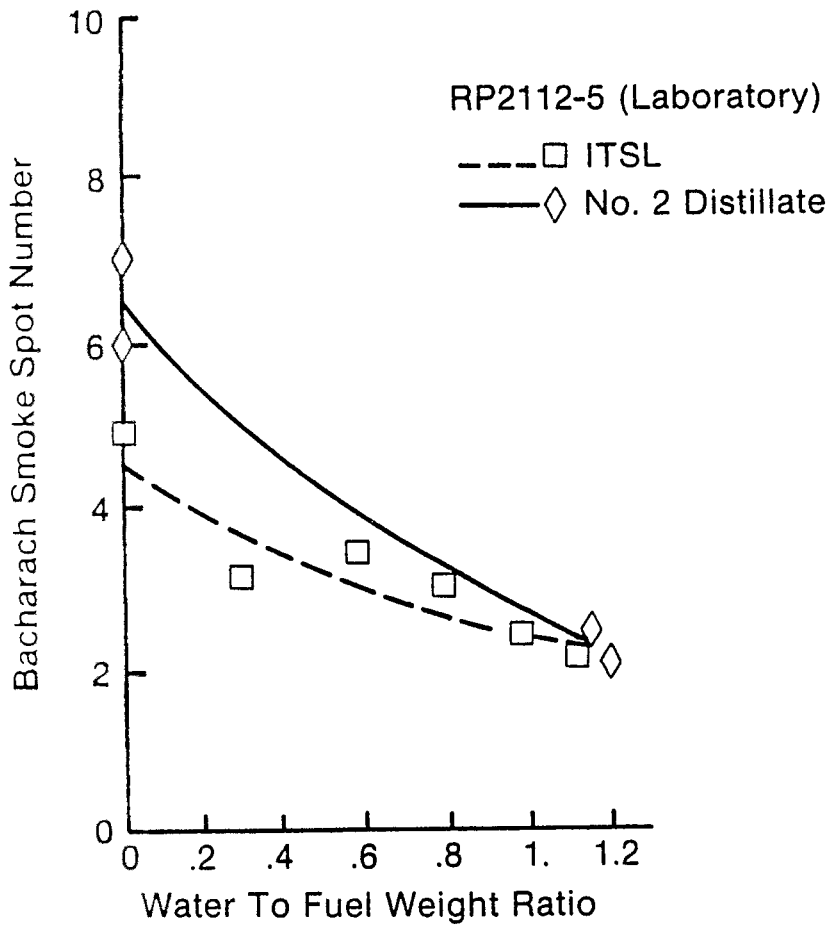


Figure 4-23. Effect of Water Injection on Smoke Spot Number (at 100% Load)

## 5. CONCLUSIONS

The conclusions reached from the ITSL CDL test program to determine the acceptability as a utility combustion turbine fuel are summarized as follows:

- The ITSL fuel is an acceptable coal-derived liquid fuel for electric utility combustion turbines.
- The characterization of the ITSL fuel viscosity vs. temperature indicated the need to heat the fuel to about 110°F to assure good atomization in the combustor. This caused no problem during laboratory testing.
- The concentrations of trace metals (sodium, potassium, vanadium, etc.) that cause high temperature corrosion of vane and blade materials are low and well within the allowable limits permitted in present combustion turbine liquid petroleum fuel specifications.
- The ITSL fuel system operation using the laboratory fuel storage, forwarding, heating, control and metering systems was uneventful; no fuel handling difficulty was experienced.
- The combustor operating on ITSL CDL fuel did not differ significantly in performance from the baseline No. 2 fuel oil operation. The effects of water injection were also similar for the two fuels.
- The increased flame luminosity in the primary combustion zone (without water injection) increased the combustor wall temperatures as was expected. The ITSL CDL wall temperature test data correlated well with the prior data; it extended the useful data base available to evaluate low hydrogen content fuels as acceptable combustion turbine fuel.
- The emissions ( $\text{NO}_x$ , CO, UHC,  $\text{CO}_2$ , and  $\text{O}_2$ ) characteristics of the products of combustion when burning ITSL CDL fuel (with 0.13% wt FBN) were consistent with those found during the engine testing of H-Coal and EDS CDL fuels. The laboratory data, correlated well with the prior data. The reduction in  $\text{NO}_x$  by water injection was also correlated with the equivalent prior data.

The ITSL CDL test program, as with the engine test program using CDL fuels, showed that the CDL fuels to be acceptable as combustion turbine fuels. This statement is based on a very short periods of operation of the storage, fuels forwarding and flow control systems during both the laboratory and the engine tests. The long term CDL compatibility and stability problems, if any, with materials currently used in the combustion fuel distribution systems, and in supporting fuel storage and forwarding systems, were not addressed. When the CDL fuels become commercially available and cost competitive for electric utility usage, long term effects of the CDL on fuel

storage and supply systems must be evaluated. Such evaluations could first be done by testing on a laboratory scale, followed by field evaluations.

## 6. REFERENCES

1. Evaluation of Coal Liquids as Utility Combustion Fuels, Palo Alto, Calif.: Electric Research Institute, December 1984. AP-3670
2. Gas Turbine Combustor Performance on Synthetic Fuels, Volumes 1 and 2. Palo Alto, Calif.: Electric Power Research Institute, June 1981. AP-1623