TABLE 5 PRODUCT GRAVITIES AND WEIGHTS

			weight, lbs		
	API	SpGr	Gross	Tare	Net
P67-69-1 (TLP Drum 1)	-0.6	1.0810	29.8	3.4	26.4
P67-69-2 (TLP Drum 2)	0.7	1.0703	149.6	15.8	133.8
P67-69-3 (TLP Drum 3)	2.1	1.0591	418.0	40.8	377.2
P67-69-4 (TLP Drum 4)	2.3	1.0575	345.0	40.8	304.2
P67-69-5 (TLP Drum 5)	3.4	1.0489	107.4	15.8	91.6
P67-69-6 (TLP Drum 6)	6.5	1.0254	301.6	40.8	260.8
P67-69-7 (TLP Drum 7)	6.9	1.0224	65.7	15.8	49.9

GC analyses were attempted on two of the early hydrotreated products on PARC's HP-6890 GC using a 150 meter Petrocal column and an FID detector. The elution times on this column have been characterized for tetralin, decalin, naphthalene, methylnaphthalene and all eight isomers of dimethylnaphthalene using pure compounds. For the same column the elution times of higher substitute methyl naphthalenes are known approximately and are consolidated into groups as tri, tetra, penta and hexa-methylnaphthalenes. It was found that the hydrotreated decant oil is primarily composed of multi-substituted naphthalenes and higher boiling, more complex components which our system cannot identify. Further hydrotreated products were therefore not analyzed.

Task 2. Evaluation of Coal-based Gasoline and Diesel Products in IC Engines and Related Studies

By introducing coal-derived streams into the refinery, several perturbations to the quality and quantity of refinery streams may result and directly impact vehicular fuels production. The coal contribution to the refinery streams will affect the quality, composition and performance of the resulting vehicular fuels. The fraction of the hydrotreated streams that boils below 180°C will be directed to the gasoline pool. Having components from coal is expected to boost octane number and aromatic content, and therefore, boost value. The >270°C cut of the hydrotreated stream would be low in sulfur due to the severe hydrotreatment. The effect on flash point will need to be determined if this stream is sent to the fuel oil pool and/or diesel pool. If this stream is combined with diesel fuel, it will add cycloparaffins, which will increase energy density [25] and boost value. However, the impact on cetane number and sooting tendency is unclear. The following task structure will permit assessment of the impact of refinery integration of JP-900 production on gasoline and diesel fuel.

Subtask 2.1. Impact on Gasoline Quality and Performance

Under this subtask, our efforts have focused on preparation of facilities for the SI engine testing activity. So, the majority of the progress to report is on Subtask 2.1.1.

Subtask 2.1.1. Preparation of Laboratory and Instrumentation

Under this subtask, we have acquired and installed the Ricardo Hydra single-cylinder research engine for use under Task 2.1.2. At present, we continue work on instrumentation and facilities hook-up to the engine test stand. Electrical power has been provided to the dyno controller. Connections were completed between the dyno controller and the operator console. We are working on two additional steps to reach the point where the engine can be operated. One is supplying cooling water to the engine stand for oil and engine coolant temperature control. The other is building a data acquisition and computerized operator interface. Chevron Texaco provided a Digalog "Cellmate" engine data system with the Ricardo engine stand, but the Cellmate is not functional and is no longer supported by Digalog. So, we are configuring our own data system based on National Instruments hardware and Labview software.

Figure 2 shows the Ricardo Hydra single-cylinder research engine in the laboratory at the Energy Institute. **Figure 3** shows the modified fuel delivery system for the ignition quality tests.

Figure 2 Ricardo “Hydra” Single-Cylinder Research Engine and Bedplate in the Diesel Combustion and Emissions Laboratory

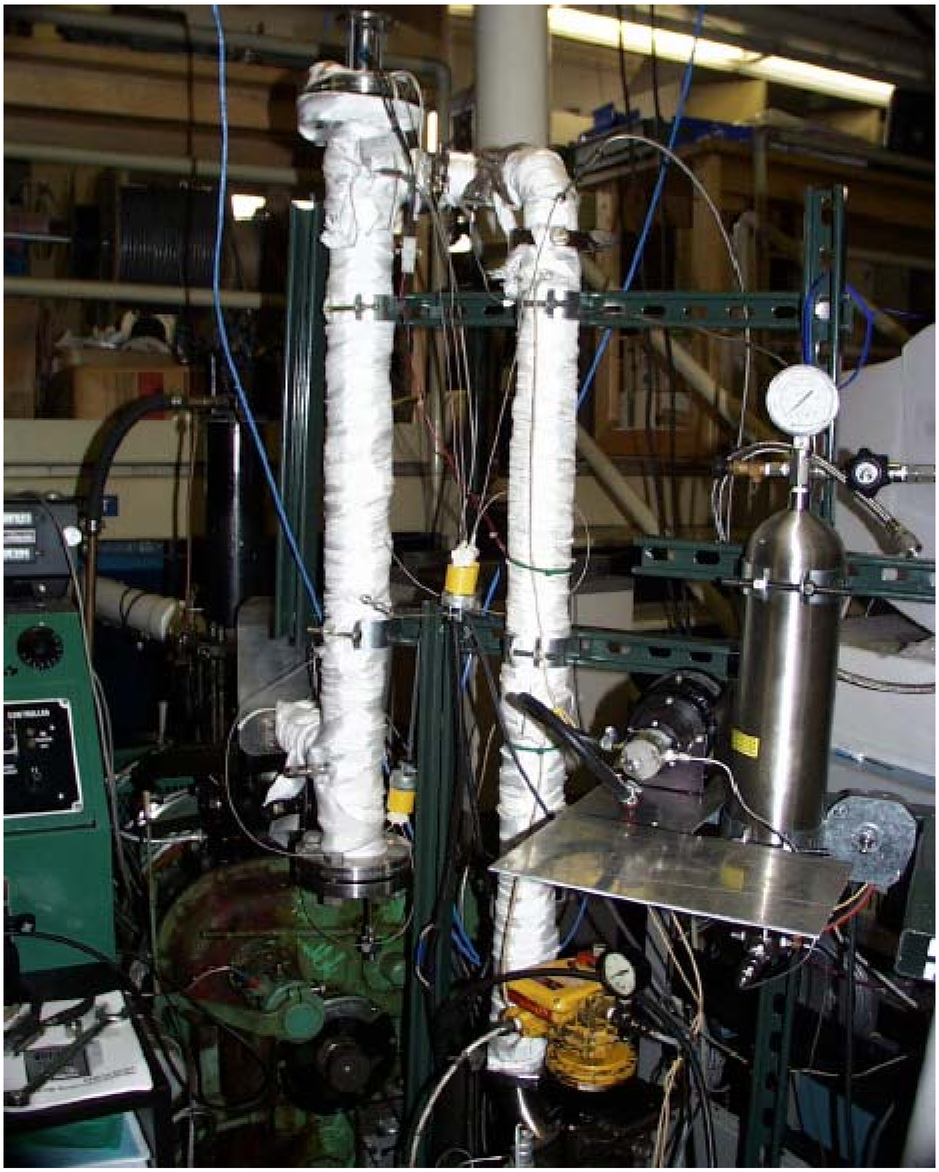

Figure 3 Fuel Delivery Apparatus to Provide Premixed Prevaporized Fuel Samples to the CFR Octane Rating Engine for Ignition Studies

Subtask 2.1.2 Impact on Chemical and Physical Properties

Under this subtask, detailed chemical analyses of fuel samples were performed. From several runs at PARC, fuel fractions were provided representing the gasoline and diesel fuel cuts. The fuel cuts were subjected to GC-MS analysis to determine the representative major compounds that could be used as surrogates in model compound mixtures. For the gasoline cut, the prominent coal-derived species are methyl cycloheaxne, decalin, propenyl benzene and tetralin (only a small amout of tetralin was detected). The impacts of these fuels on knocking tendency of base gasolines will be one of the studies we will perform in the next quarter.

Subtask 2.1.3 Impact on SI Engine Emissions and Performance

Since the work to date has focused in facility preparation, no data is available yet on this subtask. However, one aspect of preparation for Task 2.1.3 has been acquisition through a generous donation from Chevron Texaco of an AVL emissions analyzer for use on this project. That emissions analyzer was in good shape, but is presently being serviced and upgraded by AVL. It will provide an excellent and important expansion of the emissions testing capabilities available to this project.

Subtask 2.2 Impact on Diesel Fuel Quality and Performance

Under this subtask, we have focused on two activities, both related to facility development. One side of the work has been refinement and enhancement of two existing engine test stands, one housing a Navistar V-8 7.3L turbodiesel engine and the other housing a DDC 4-cylinder 2.5L turbodiesel engine. The other activity has involved developing ignition testing capabilities which involved purchase of new IQT instrument and development of an ignition test capability as an expansion of an existing CFR Octane Rating Engine.

2.2.1 Acquisition, Installation and Instrumentation of Ignition Test Equipment

At present, we await the arrival of a new "IQT" ignition quality test instrument. The instrument should ship to Penn State very soon. A research staff member and a graduate student visited the vendor to receive training on the instrument, which was included in the purchase on the instrument. Facilities connections for the device for ventilation and electrical service have already been prepared.

In addition, a device to provide premixed prevaporized fuel samples to be fed to a CFR Octane Rating engine, operated with the spark plug deactivated, has been configured to serve as a "rapid compression machine" to study the elementary effects of fuel composition on the ignition process of hydrocarbons. Some preliminary data has been obtained for reference fuels and is presented below. **Figure 4** provides a sample of the type of data this experiment can provide. Here the ignition of n-heptane is examined, at fixed inlet temperature and equivalence ratio (0.05) and with increasing compression ratio. In **Figure 4(iii)** the first evidence of 1^{st} stage ignition is observed at roughly 680 K. In **Figure 4(iv),** 2^{nd} stage ignition begins at roughly 800 K. These results are consistent with published experiments and numerical simulations of n-heptane ignition.

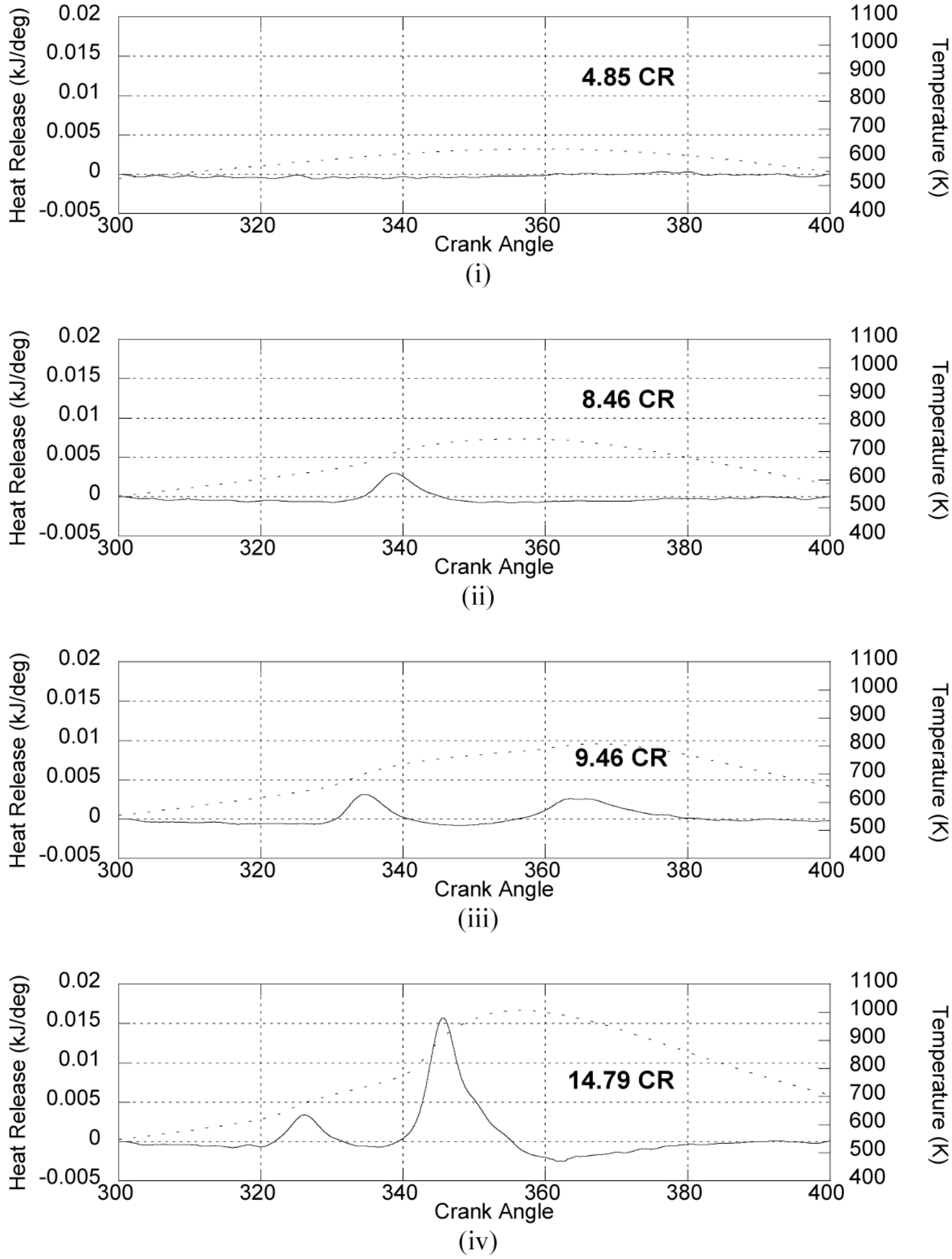

Figure 4 Ignition Process for n-Heptane at ϕ=0.05 and Increasing Compression Ratio. In Plot (iii) the First Evidence of 1st Stage Ignition is observed at roughly 680 K. In Plot (iv), 2nd Stage Ignition Begins at roughly 800 K.

2.2.2. Development of Analytical Methods and Test Procedures

The "IQT" apparatus is now covered under an ASTM test method so that its operation and application are considered standard practice. We have agreed to participate in round robin testing activities to help support the community's use of the IQT and to provide external comparison of our data.

The modification of the CFR Octane Rating engine to serve as a rapid compression machine for ignition studies represents a unique adaptation of a standard instrument and will provide a means of comparing experimental data with kinetic models of the ignition process.

2.2.3. Evaluation of Capabilities and Needs for Supplemental Measurements and Analyses

The analytical methods developed for the characterization of the fuel cuts from the PARC runs can now serve as the basis for subsequent fuel and SOF chemical analyses. We have also begun to develop procedures for use of an existing FTIR spectrometer to speciate the products of our ignition tests, so that we can detect the intermediate species present as we pass through first and second stage ignition.

2.2.4. Impact on Chemical and Physical Properties

At present two studies are underway. Both are based on the speciation of the diesel cut from the PARC run. The GC-MS data showed that two prominent and representative compounds were fluorene and phenanthrene. So, baseline diesel fuels are being doped at 1 to 5 wt.% to simulate the diesel fuel. In one study, engine emissions tests are being performed at Southwest Research Institute through a Penn State graduate who is spending at year at SwRI as an intern. In the other study, a undergraduate student is performing smoke point tests on doped diesel fuel samples to assess the impact of these coal-derived compounds on the sooting tendency of the diesel fuels. Data from both of these studies should be available by mid-April 2004.

2.2.5 Impact on CI Engine Emissions and Performance

For the purpose of better understanding the impact of the coal-derived compounds on the injection, ignition and combustion of diesel fuels in a practical engine, we are developing an installation of an existing AVL 513D Engine Videoscope (purchased under an NSF Research Equipment Grant, # CTS-0079073) in our Navistar V-8 7.3L turbodiesel engine. This requires machining access for an endoscope probe and a light guide to visualize the fuel spray and the spray flame.

In parallel, we are adding instrumentation to an existing DDC 2.5L turbodiesel engine for examination of the impact of fuel composition of combustion and emissions. The instrumentation includes an AVL Indimodule combustion analysis system, which will permit highly accurate (true simultaneous) acquisition of fuel rail pressure, injection timing and cylinder pressure. At present we have received the Indimodule hardware and are waiting to receive the pressure probe and custom machined glow plug mounting adapter for the pressure probe. In addition, we will be meeting in late March 2004 with a