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PROGRESS ON MIDDLE DISTILLATE COMBUSTION RESEARCH PROGRAM AT THE COMBUSTION AND CARBONIZATION RESEARCH LABORATORY

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Presented to the Committee on Middle Distillate Fuels
at the Canadian General Standards Board Committee Meetings,
April 1989, Edmonton, Alberta.

ENERGY RESEARCH PROGRAM
ENERGY RESEARCH LABORATORIES
DIVISION REPORT ERL/ERP 89-72(OP)

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by

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ABSTRACT

A brief account of progress summary on the Middle Distillate Fuels Research Program at the Combustion and Carbonization Research Laboratory is reported. The report describes the program initiation process, significant developments, and current efforts being made to transfer the technology to the Canadian oil industry. A list of technical reports, computer programs, and publications resulting from this research program is also given.

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BACKGROUND

Ever-increasing global energy demand and depleting conventional resources continue to press the oil industry for action on energy conservation, as well as for exploration for new fossil fuel supplies. Since the energy crisis of the seventies, the industry has generally responded to reflect the changes in energy demands. The product yield from the crude barrel is now incorporating heavier distillate cuts; synthetic distillates have been produced from unconventional sources such as oil sands and heavy crude. However, degrading feedstock quality and stringent environmental regulations restrict the use of such fuels to some extent. Operational requirements of equipment presently in use may not be compatible with these fuels, which often have different characteristics that are not covered under current specifications. For example, synthetic distillates contain higher proportions of aromatics, compared to conventional distillates, and these aromatics are known to generate higher particulate emissions in combustion equipment. The introduction of these fuels has created a need for suppliers and users to reexamine the design methodologies and expected performance characteristics of lower grade products. Product evaluations of these fuels have been carried out by major manufacturers of turbine and diesel engines [1-2], with similar research activities being carried out in other areas. Product performance evaluation is equally important in residential combustion appliances since appliance safety and reliability along with environmentally acceptable emissions must be ensured.

The Canadian oil industry faces a greater challenge ahead since Canada's per capita energy consumption is one of the highest in the world. It is possible that, within 6-10 years, more than half of Canada's total domestic production will be derived from the oil sand bitumens, heavy crude and heavy oil deposits from Western Canada. This scenario reflects a practical solution to Canada's energy needs, but it does require technology development and performance evaluation to ensure safe and efficient utilization of these fuels in existing appliances. Performance evaluation of a variety of lower grade fuels in residential combustion appliances can be performed in a controlled laboratory and efficient combustion technologies can be explored. Such practical information will be beneficial to the oil industry, allowing greater blending flexibility and product control for cost saving. The standards writing bodies and regulatory agencies require such information to update the existing fuel specifications, relating to changes in product quality and equipment requirements.

The Canadian General Standards Board (CGSB) established a task force under the Heating Fuel Panel of the Committee on Middle Distillate Fuels in 1982 (Can 2-3.2). This coincided with the request for guidelines applicable to refinery operations from a specific company, that had experienced field problems with high aromatic fuels. The committee members agreed to assign a comprehensive combustion evaluation of middle distillate fuels covering a wide range of properties and crude sources. Members believe that such a program could lead to the development of a fuel indexing system that will allow ranking of fuels according to their properties. Prediction of fuel performance could be made using this index information without actually performing laboratory testing. This perceived system was tentatively defined as "burnability index" by the members. The Combustion and Carbonization Research Laboratory (CCRL) was requested to carry out this research program and the industry agreed to contribute distillate fuels for testing.

SIGNIFICANT DEVELOPMENTS

EXPERIMENTAL FACILITIES

(a) Development of experimental program for fuel performance evaluation

In 1983, the Energy Conservation Technology (ECT) Section of CCRL designed a laboratory rig and developed an experimental program to evaluate the combustion performance middle distillates. The development was successfully completed a year later. Detailed information on the progress of CCRL program was reported to representatives of the Canadian oil industries, including CGSB members at the annual meeting of the Ontario Petroleum Association (A) and at subsequent CGSB committee meetings (B). Similar presentations were made to other research organizations (C,D).

The laboratory equipment includes two commercial warm-air domestic furnaces, a chilled air distribution system, temperature-controlled fuel conditioning unit, continuous emission analyzers, and automated data acquisition and processing units. Special emphasis was given to the design of the system to simulate the actual environment of a residential heating appliance. Figures 1 to 4 illustrate the experimental equipment and the outline of the experiment. The CCRL program has been reported in a number of publications (1-2).

(b) Calibration of a continuous smoke meter for particulate measurement

A commercial smoke opacity meter designed for determining particulates from diesel engine exhaust gases was specially calibrated and a procedure was developed to determine transient particulate levels from residential oil burners. Opacity readings were correlated with industry standard Bacharach smoke test numbers and actual mass of soot for specific fuels.

(c) Video recording of combustion flame characteristics

The experimental rig also has a video camera located above the heat exchanger, for recording the actual dynamic flame characteristics in the combustion chamber through a heat-resistant quartz window. A schematic of the video set-up is shown in Figure 5.

TEST FUELS

(a) Supply

The following Canadian oil companies and organizations contributed the distillate fuels for the CCRL fuel evaluation program:

- Esso Petroleum Canada, Sarnia refinery;
- Petro-Canada, Edmonton and Oakville refineries;
- Shell Canada Ltd, Oakville refinery;
- Suncor;
- Texaco Canada Ltd;
- Ultramar Canada Ltd, Quebec City refinery;
- National Research Council of Canada, Department of Mechanical Engineering, Fuels & Lubricants Laboratory.

(b) Fuel variety

Forty-nine fuels were evaluated. They included 9 furnace fuels, 9 diesel fuels including projected future compositions, 5 light cycle oils, 5 synthetic distillates, 1 jet fuel, and 20 CCRL-developed blends. The CCRL blends were prepared to obtain fuels with specific levels of such properties as viscosity and aromatics, using the distillates contributed by oil companies as blending stocks. This extended the range of fuel properties not normally available from the refineries.

DETERMINATION OF FURL PROPERTIES

(a) Standard analysis methods

Each fuel was analyzed for the following physical and chemical properties: aniline point, cloud point, flash point, pour point, calorific value, density, distillation range, viscosity, aromatics, saturates and olefins by fluorescent indicator adsorption (FIA) and mass spectrometry (MS), aromaticity by nuclear magnetic resonance (NMR), Ramsbottom carbon residue, water and residues (BSW), and ultimate analysis. Analyses were performed by the Fuels Characterization Research Laboratory of CANMET's Energy Research Laboratories, using standard ASTM methods. A report was prepared and submitted to CGSB Committee on Middle Distillate Fuels (3). Selected samples were later analyzed for aromatics by supercritical fluid chromatography (SFC). Detailed structural characterization was performed on selected fuels and results were published in the literature (4).

(b) Development of a new method for determining aromatics in diesel fuels and heating fuels

During the course of the performance evaluation study, it became apparent that a reliable analytical technique for determining fuel aromatics was critical for accurate interpretation of combustion performance. A general consensus from the oil industry indicated an increase in demand for a hydrocarbon-type analysis that could handle different refinery products, as well as a requirement for analytical methods which were applicable to materials with wide boiling ranges (4). These requirements have led to the development of a new analytical technique utilizing supercritical fluid chromatography (SFC)(5). The SFC method provides simple chromatograms as shown in Figure 6. This technique was first proposed to the Canadian General Standards Board (CGSB) in October 1987 (F), for consideration as a standard for total aromatics in liquid petroleum fuels. A draft proposal was submitted to the Middle Distillates and Petroleum Test Methods Committees in March 1988 (6). A copy of the method, as published in an American Chemical Society journal (7), was distributed to committee members in April 89. The Energy Conservation Technology Section of CCRL also contributed other related publications to the literature (8,9).

This SFC method has significant adventages over the FIA method in terms of analysis time, method reliability, improved analytical instrumentation, and applicability to coloured and high boiling fuels, such as in distillates from non-conventional crude. The SFC method extends the final boiling range to a maximum of 450°C from FIA's maximum limit of 315°C. The long analysis time required by FIA, about 5 to 7 hours per sample, can be reduced to between 15 and 45 minutes by using SFC. The CGSB Committee on Petroleum Test Methods commissioned a preliminary round robin study of the proposed SFC method in 1988. The study was completed in March 1989 and a report was forwarded to CGSB (10).

(c) Determination of mono-, di-, and polyaromatics in distillate oils

Analytical technologies for determining different aromatic compounds such as mono-, di-, and polyaromatics suitable for refinery application are being investigated. Low resolution mass spectrometry, NMR, and ultraviolet (UV), and SFC techniques are included. Results were reported in an American Chemical Society publication (11). A joint project on the development of aromatic hydrocarbon type analysis using SFC is being carried out by the Energy Research Laboratories and the Alberta Research Council. The project is expected to be completed by the end of 1989.

CORRELATION OF FUEL PROPERTIES AND COMBUSTION PERFORMANCE

(a) Combustion characteristics

For each fuel evaluated using the CCRL program, the following burner performance characteristics were determined: burner ignition behaviour such as pulsation, sound, delayed ignition, failure; video flame characteristics; transient and steady state emissions of particulates, oxygen (O_2), carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x), and hydrocarbons (HC); flue gas temperature; excess air; steady state efficiency; and temperature differential between cold air return and warm air plenum. A typical experimental run included an one hour steady state operation followed by 5, 10 minute on/off cycles.

(b) Combustion data processing and method of reporting

The experimental program provides profiles of emission concentrations recorded over the entire run. There are three critical phases: startup transient (cold start), mid-run steady state, and shutdown transient. Emissions are recorded and processed individually for each phase. A typical profile of CO emissions is shown in Figure 7. Cold start and shutdown emission data are calculated on a mass basis, as milligrams of CO per transient peak, derived from the area under the corresponding volumetric peak. Cyclic emissions are calculated similarly for five cycles and mean data for each transient operation are reported. The same calculations apply to hydrocarbon emissions, which show profiles similar to those of CO. For particulates, continuous recording of smoke opacity meter shows transient peaks (cold start and cyclic starts) as reported in Figure 8. Maximum opacity at the peak height was provided by the digital output of the meter and and area under the peak was measured on the recording paper. Both data were used in combustion data analysis.

Property/performance correlation plots were prepared to determine specific relationships between fuel properties and combustion characteristics. Cold start transient emissions and average cyclic transient emissions show significant differences in emission concentrations as shown in Figure 9. This appears to be a direct reflection of the temperature effect on combustion; cold start operations are affected by cold fuel (nozzle oil temperatures of 17-20°C) and environment, whereas the cyclic operations experience favourable warm conditions (nozzle oil temperature of 40-75°C). It suggests that cold start combustion is critical and that a low grade fuel should be able to produce a favourable cold start in order that combustion can be sustained for normal operation. Partial discussions on these correlations were published elsewhere (12) and presented to industry representatives (I).

(c) Predominant fuel properties

Correlation data indicate that, among the various fuel properties, fuel viscosity and fuel aromatics show the strongest influence on performance characteristics (Figures 10 and 11). An increase in viscosity or aromatics in fuels produces higher levels of particulate and gaseous emissions, and poses a higher possibility of burner ignition problems in residential combustion systems. Since both parameters show similar effects on combustion performance, specific experiments were carried out to isolate the effects contributed by each.

(d) Co-linearity between fuel properties

Data analysis indicates that isolation of the performance characteristics created by individual fuel property is not feasible due to the intrinsic, co-linear nature of the physical and chemical properties of distillate oils. The effect of a certain property can only be discussed under the condition that other fuel properties be specified. A minimum of three dominant properties such as viscosity, aromatics and density are to be included in data interpretation, to ensure that fuel properties are well represented. These properties are usually represented in the form of multi-linear equations.

(e) Development of an empirical equation for prediction of soot production

Initial data interpretation of property-performance correlations was hampered by the unavailability of computer software for multilinear regression analysis capable of handling co-linear parameters. CCRL developed a computer program specifically for handling co-linear parameters and has proposed an empirical equation for estimating soot production (13). This equation predicts the soot emitted in terms of smoke opacity, from a distillate fuel fired in a warm air residential combustion appliance equipped with a flame retention head burner. A brief discussion on this program was presented to the CGSB Committee on Middle Distillate Fuels in April 1989 (J).

(e) Oil droplet characterization and correlation with soot formation

CCRL has initiated a joint project with the National Research Council of Canada to study the correlation of combustion performance and characteristics of oil droplets generated at the residential burner. Oil spray characteristics of fuel oils with specific properties are being determined using laser techniques and are interpreted in relation to soot formation. The project is expected to be completed in 1990.

ACCEPTANCE OF PROGRAM BY INDUSTRY AND INFLUENCE ON SCIENTIFIC COMMUNITY

The CCRL middle distillate combustion research program receives full support from the Canadian oil industry. CCRL has been contracted by a number of oil companies to provide laboratory test results on performance of some commercial fuels and specific products. Combustion and fuel quality related technical presentations and publications have been made to national and international scientific associations. Scientists from Battelle Laboratories of Columbus, Ohio, Brookhaven National Laboratory of Long Island, New York, and the Senter for Industriforsking of Norway, along with many industrial representatives from North America have visited CCRL for advice in construction of similar facilities and for exchange of scientific information relating to oil combustion.

TECHNOLOGY TRANSFER

A one-day workshop is being planned for mid-1990 to present the CCRL program to representatives of Canadian oil companies and to standards/regulatory organizations. This technology transfer will be carried out through oral presentations, a tour of the laboratories, technical literature, a reference guide for petroleum-distillate producers and a handbook on quality characterization of Canadian distillate fuels. The reference guide contains data on the combustion performance of 49 middle distillate fuels and the combustion index system. Empirical equations for the prediction of residential appliance particulate emissions derived from basic fuel properties will be described. The handbook on fuel quality characterization provides indepth information on properties of distillate fuels from various origins and types. These technical information will provide the producer with useful guidelines and flexiblity in production, blending and marketing stretagies. Ultimately, the industry could utilize the information to predict pollution emissions from oil combustion contributed by the residential sector. This will provide vital information essential to our efforts in maintaining a sustainable environment.

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(D) Lee, S.W. " Particulate emissions from domestic oil furnaces as related to middle distillate fuel quality". Brookheaven National Laboratory. Upton, N.Y. July 8, 1985.

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ACKNOWLEDGEMENT

The authors wish to thank D.E. Barker, T.G. Sellers, F. Preto, F.L. Wigglesworth, D.C. Post, Combustion and Carbonization Research Laboratories and L. Mysak, Engineering Services, of Energy Research Laboratories and D. Sullivan of Engineering and Technical Services Division for their assistance in this program.

Generous contribution of test fuels by various oil companies is greatly appreciated.

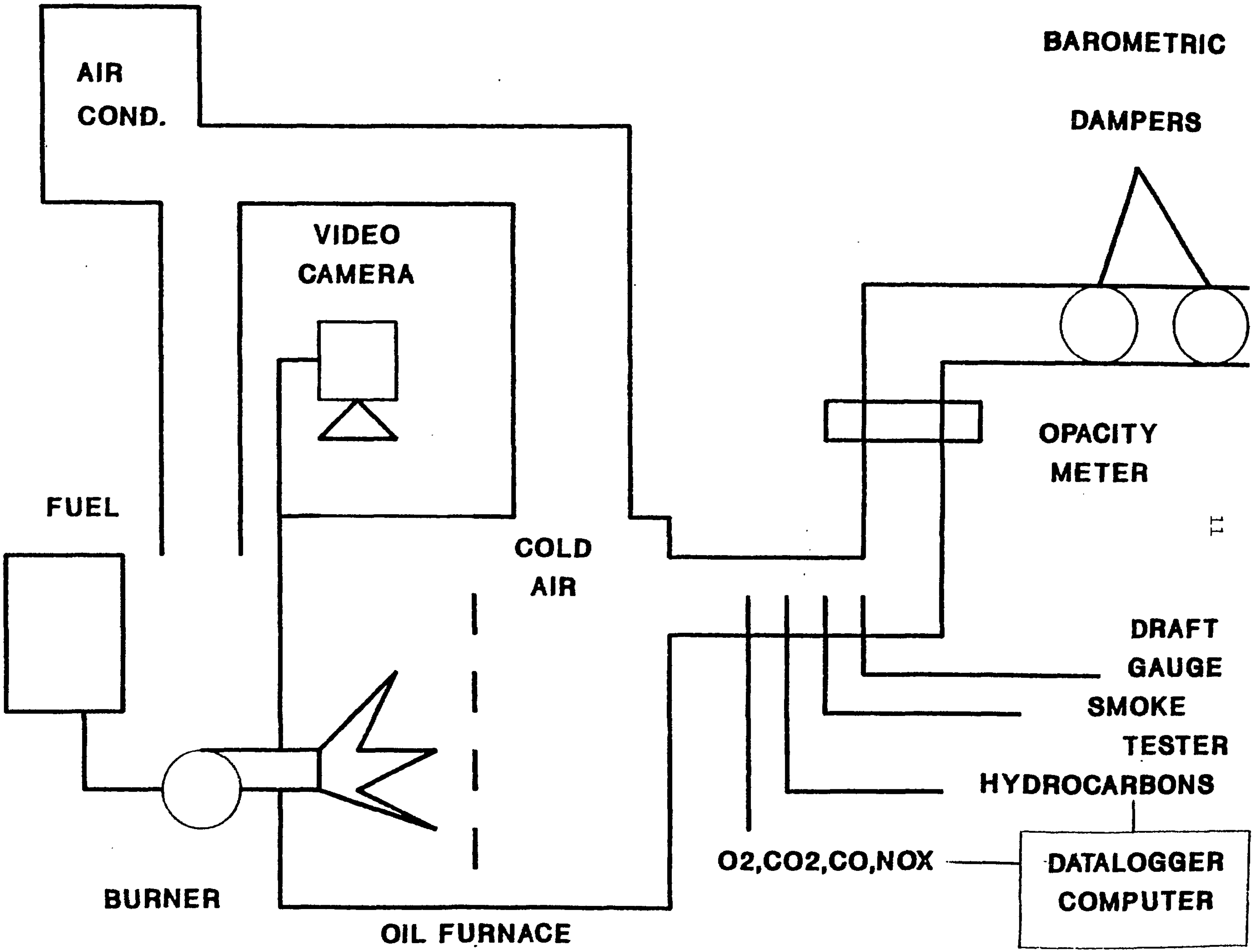

Figure 1. Experimental equipment for middle distillate fuels program

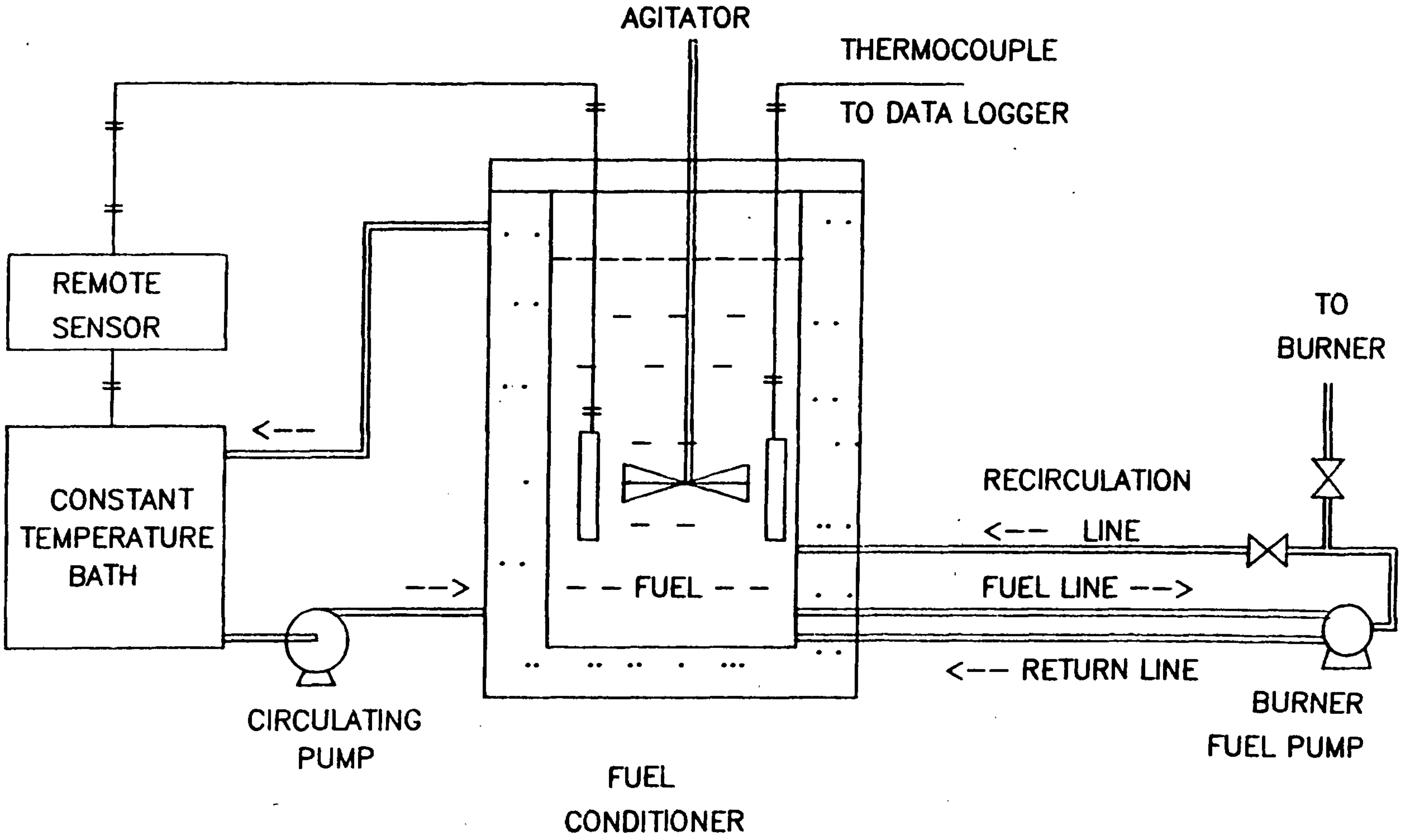

Figure 2. Fuel conditioning and supply system

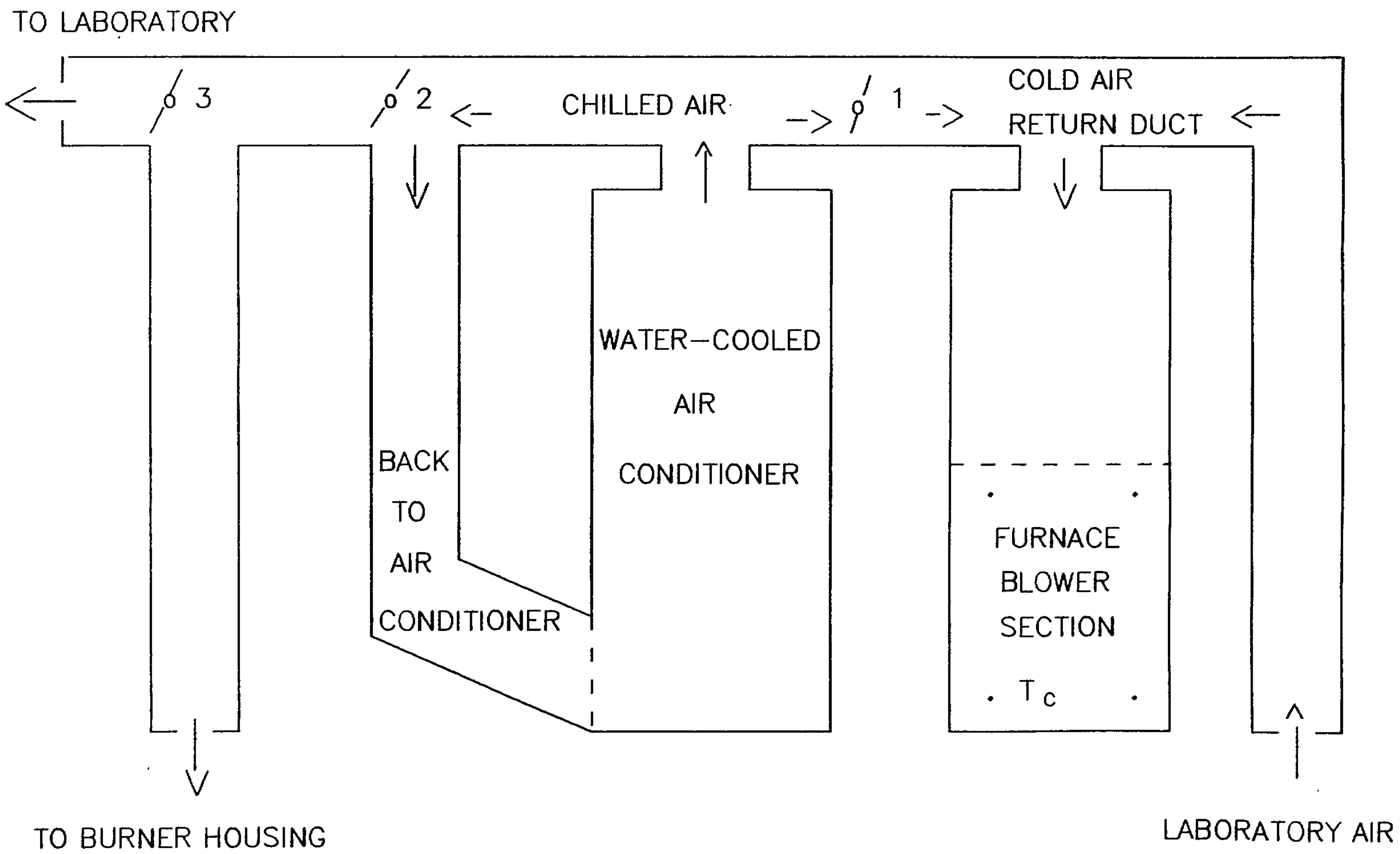

Figure 3. Chilled air distribution system

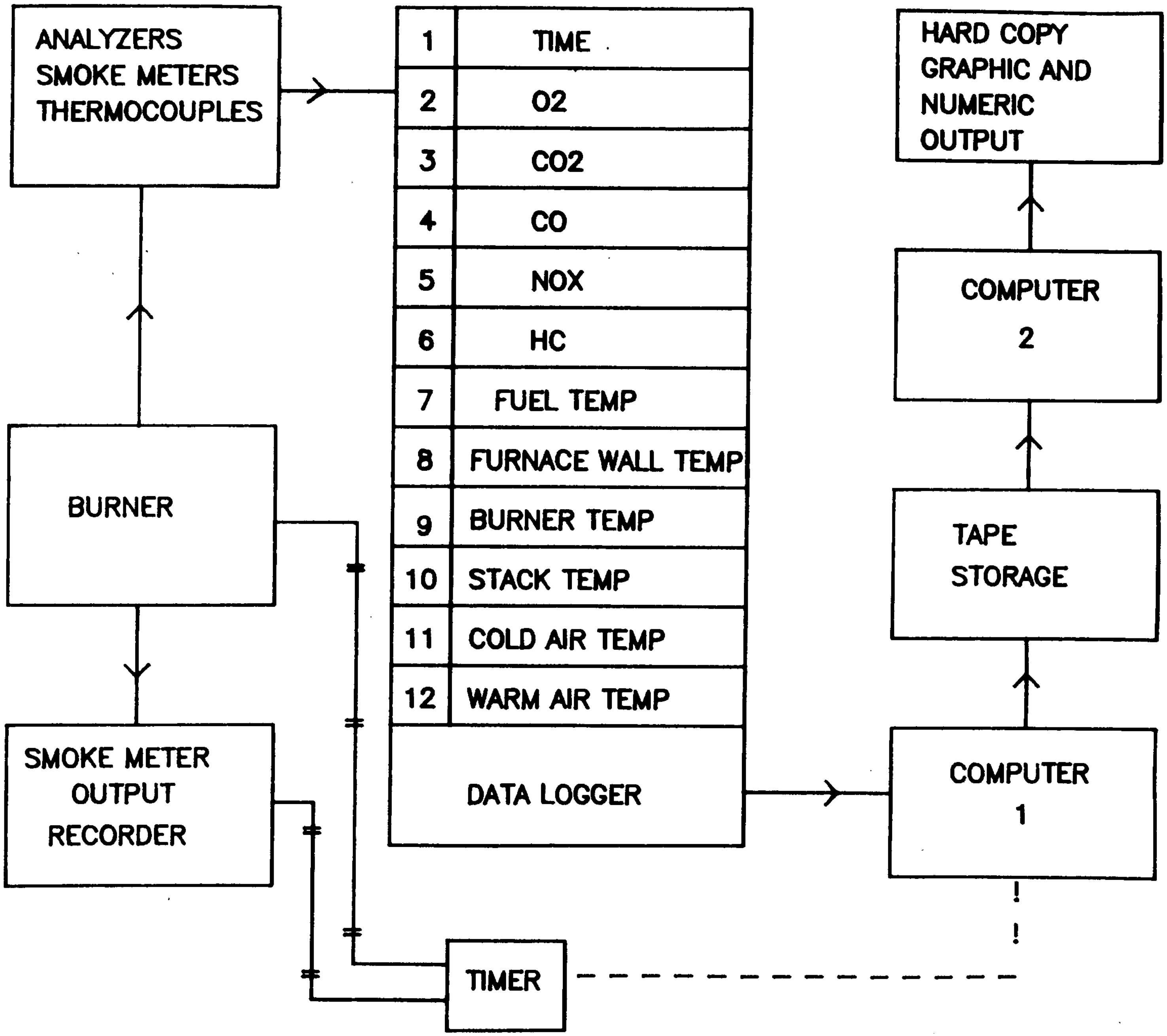

Figure 4. Data acquisition and processing schematic.

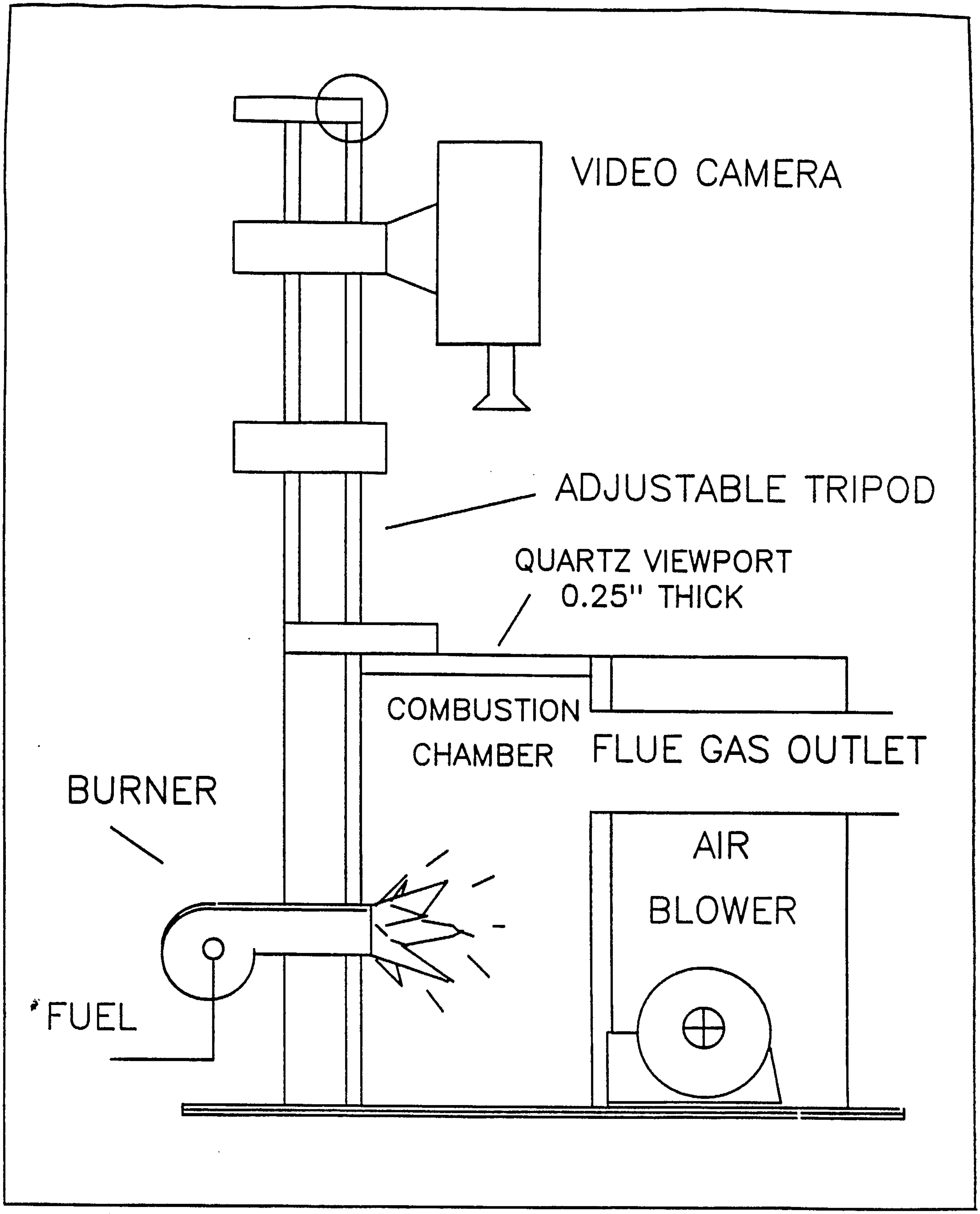

Figure 5. Heating appliance with flame video equipment

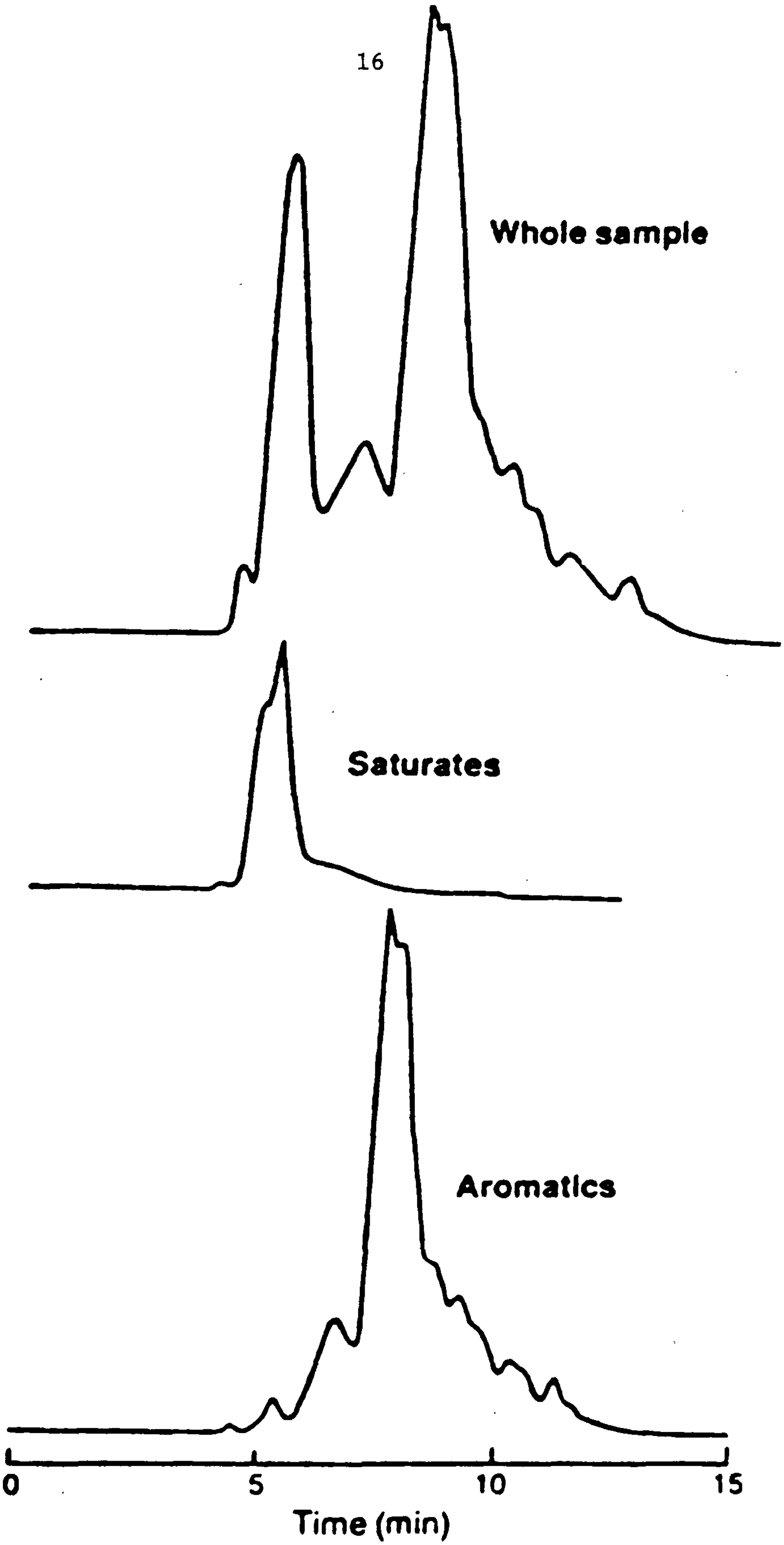

Figure 6. Typical SFC chromatogram of a commercial diesel fuel

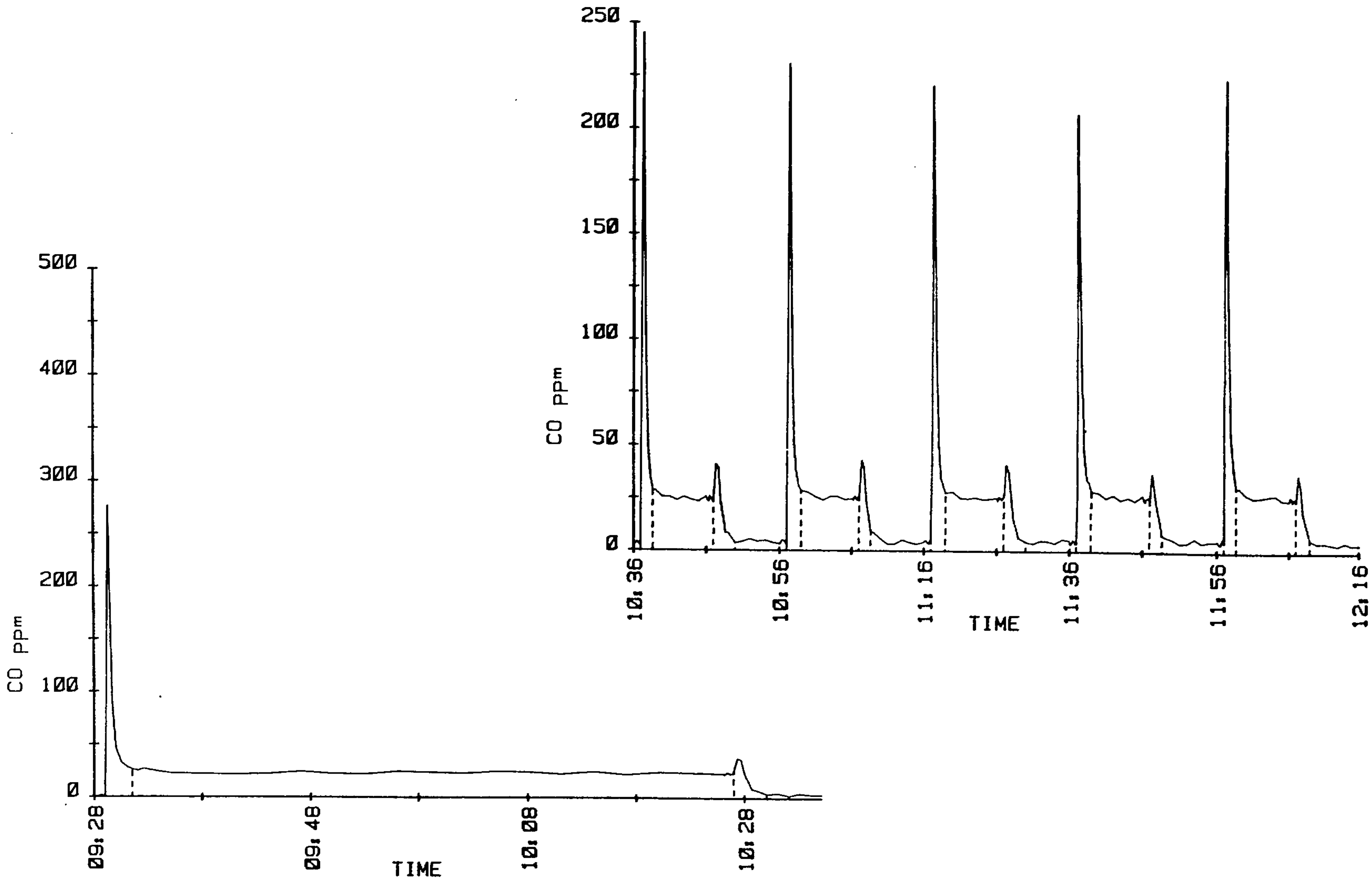

Figure 7. Typical carbon monoxide emission profile of a distillate fuel from a CCRL combustion experiment

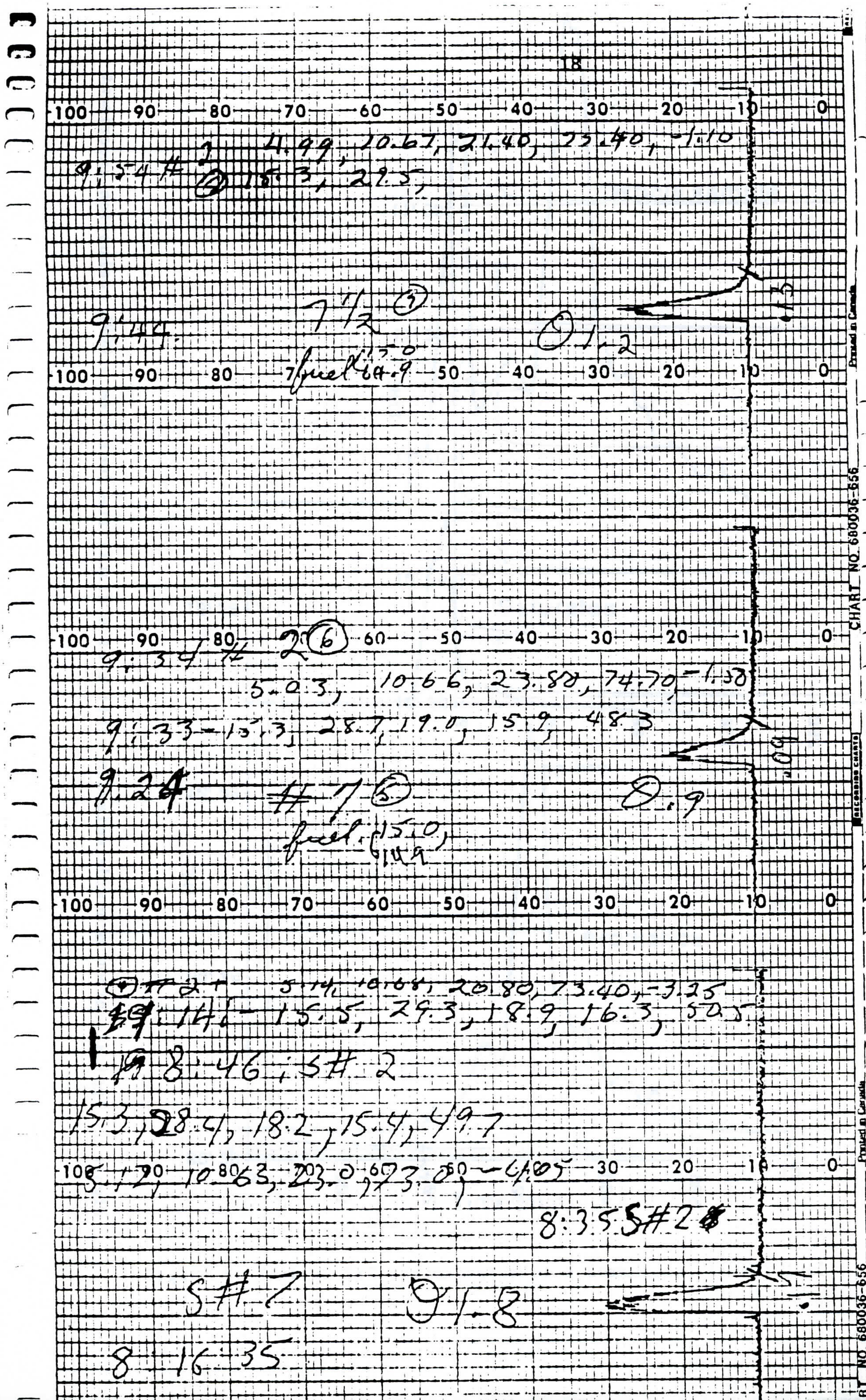

Figure 8. Particulate emissions from cold start transient and warm cyclic operations

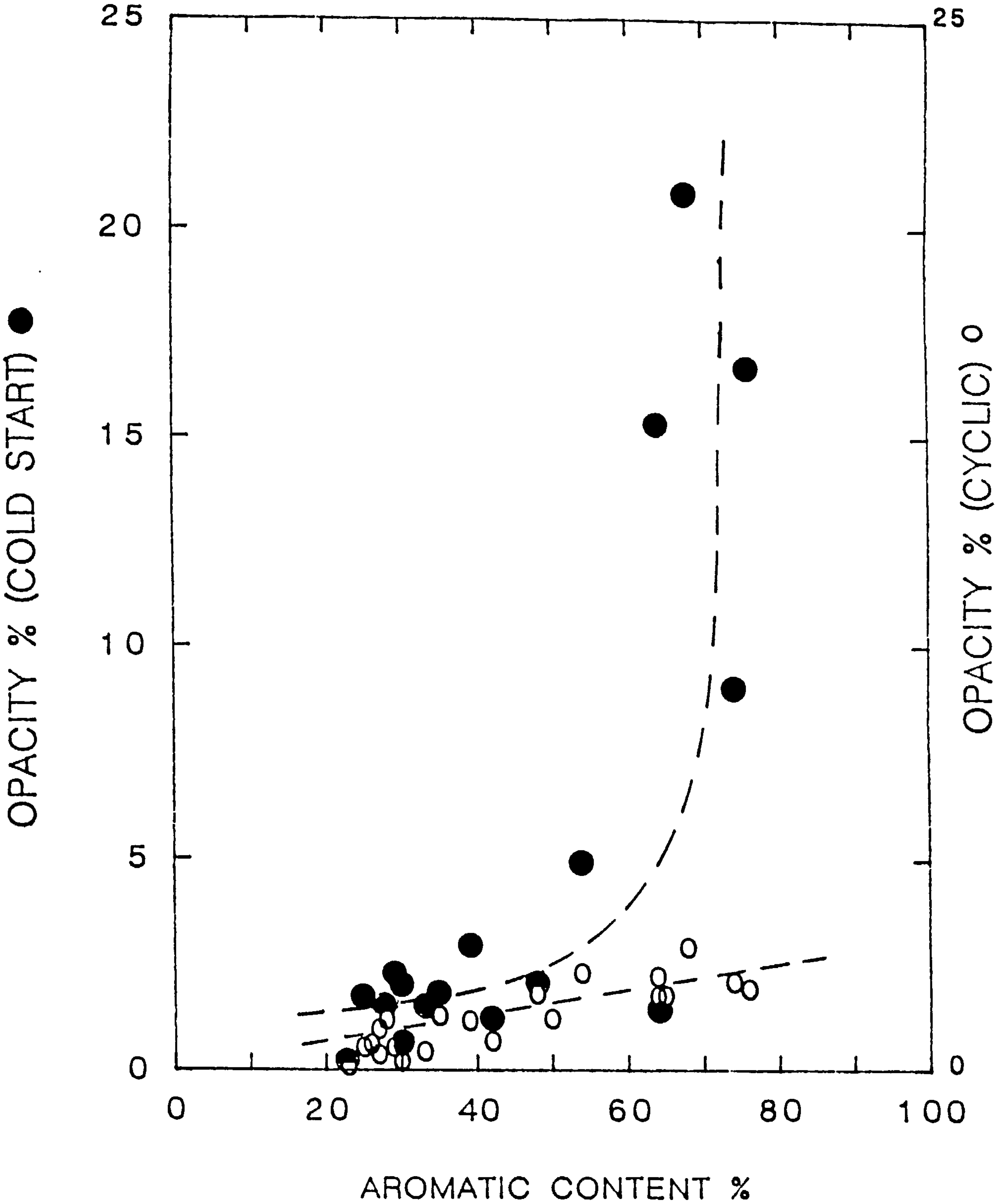

Figure 9. Effects of fuel aromatics on cold start and cyclic particulate emissio

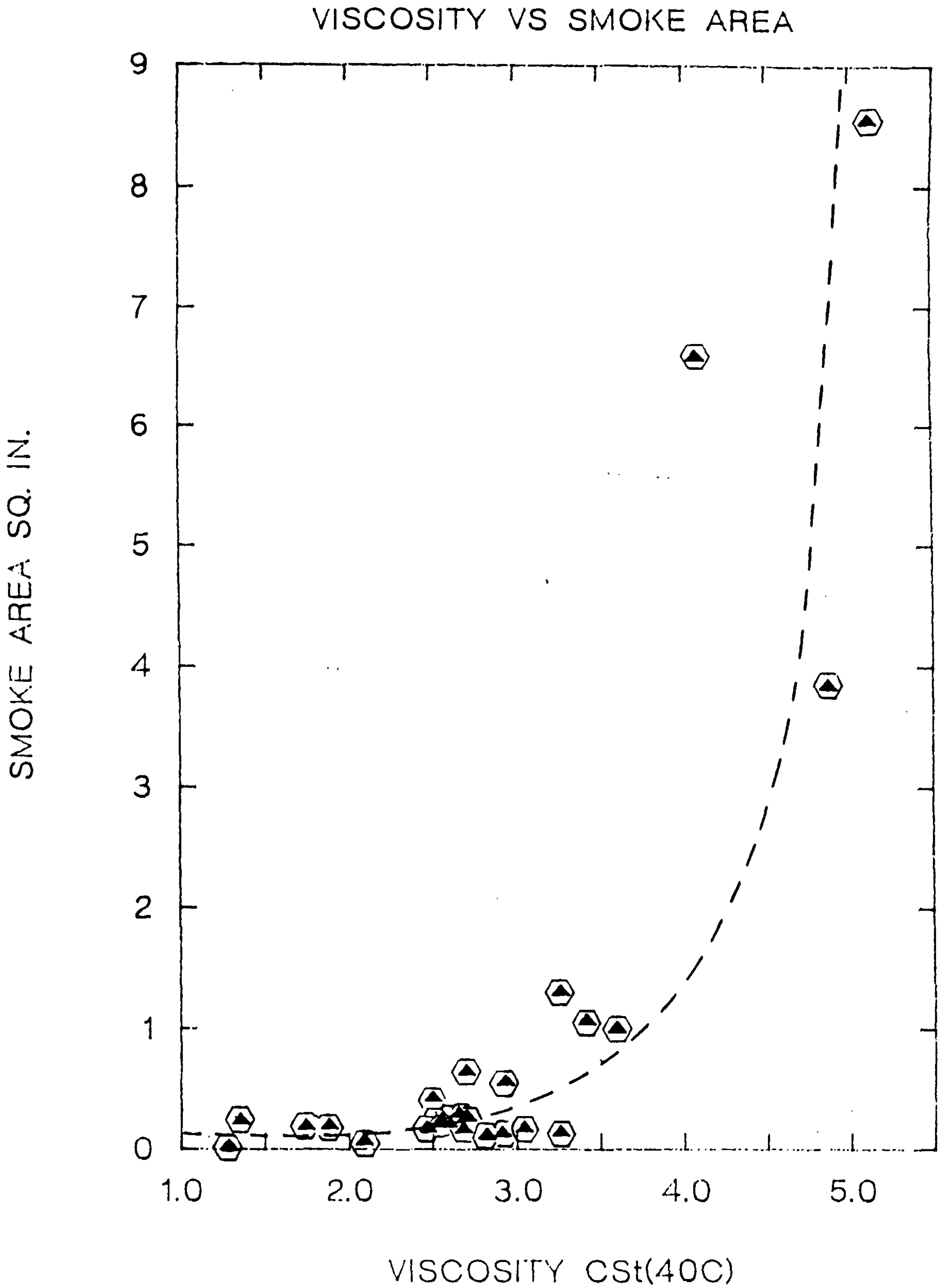

Figure 10. Correlation plot of fuel viscosity and particulate emissions

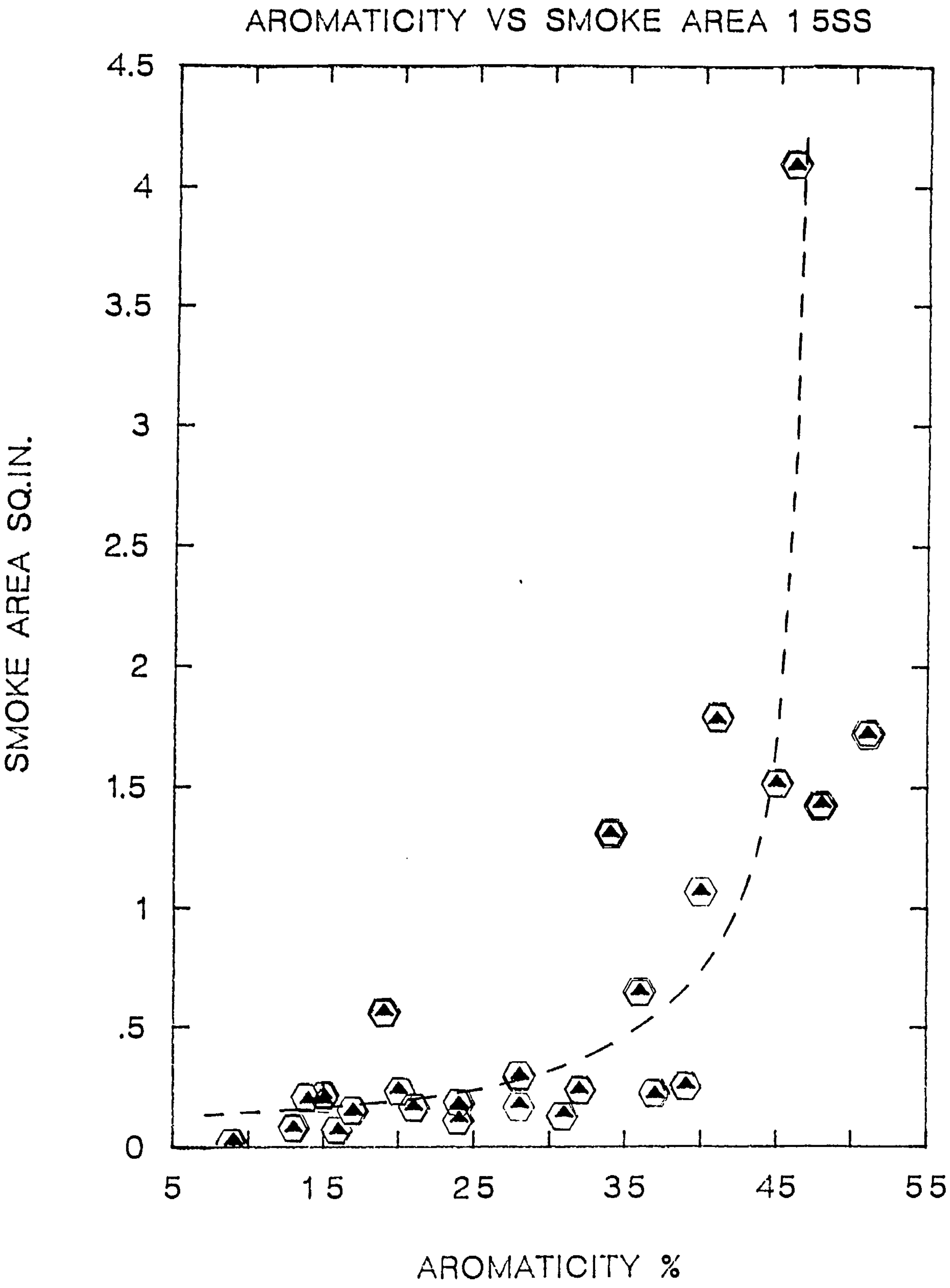

Figure 11. Correlation plot of fuel aromatics and particulate emissions