

# Analysis of Marine Diesel Fuel with the Advanced Distillation Curve Method

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## S Supporting Information

**ABSTRACT:** Ocean-going ships burn heavy fuel oil. The combustion of heavy fuel oil in marine diesel engines emits nitrogen oxides, sulfur oxides, and particulates into the air. Growing public concern over air quality has led to increased scrutiny of heavy fuel oil as a source of air pollutants, with calls for greater regulation of its composition to safeguard public health and the environment. Heavy fuel oil is a complex mixture, prepared by blending residual oil from petroleum distillation with more volatile fractions to meet industry standards. The fuel composition has a significant effect on the type and amount of combustion products produced, but the complexity of heavy fuel oil blends has hindered past efforts at analysis. The advanced distillation curve (ADC) method was developed as a complex fluid analysis protocol, combining thermophysical and chemical properties measurement. We applied the ADC method, under reduced pressure, to a sample of IFO 380 intermediate fuel oil to characterize its volatility and composition as a function of volume fraction. Applying the analytical method to heavy fuel oil yields quantitative data that can be used to model and design more efficient internal combustion engines for ocean-going ships, improving maritime fuel economy while reducing the amount of harmful pollutants released into the atmosphere.

## 1. INTRODUCTION

Maritime transport currently accounts for over 80% of global trade by volume. Over the last four decades, the volume of seaborne trade has grown by an annual average of 3.1% and is expected to double by 2033.<sup>1</sup> The majority of ocean-going cargo ships today are powered by burning heavy fuel oil in marine diesel engines.<sup>2</sup> Heavy fuel oil is a low-cost blend of residual oil from petroleum refining and distillate gas oil, which is added to lower the fuel's viscosity to meet industry standards. Residual oil contains a large fraction of the sulfurous compounds and heavy metals found in petroleum. The combustion of heavy fuel oil in marine diesel engines produces nitrogen oxides, sulfur oxides and particulates from incompletely burned fuel, and mineral ash. The establishment of emission control areas in the Baltic Sea, North Sea, and coastal waters surrounding North America reflects growing public concern over air pollution from maritime transport.<sup>3</sup> The projected growth in global maritime commerce underscores the need to reduce air pollution stemming from combustion of heavy fuel oil in the future.

The combustion of a fuel droplet in a marine diesel engine is a complex process. The physical and chemical properties of the fuel, as well as the engine operating parameters, are important factors in the overall efficiency of the process and the exhaust emission profile. Fuel droplet volatilization plays a vital role in the combustion process. For example, the formation of carbonaceous Cenospheres may be described by the boiling of volatile fractions present in a droplet of heavy fuel oil.<sup>4</sup> Measuring the changes in the physical and chemical properties of the fuel as it is heated is important in modeling the droplet combustion process, which will provide new approaches to fuel formulation and marine diesel engine design.

The Advanced Distillation Curve (ADC) is a significant improvement over earlier approaches to complex fluid characterization, featuring (1) a composition-explicit data channel for each distillate fraction (for both qualitative and quantitative analysis), (2) temperature measurements that are true thermodynamic state points that can be modeled with an equation of state, (3) temperature, volume, and pressure measurements of low uncertainty suitable for equation of state development, (4) consistency with a century of historical data, (5) an assessment of the energy content of each distillate fraction, (6) trace chemical analysis of each distillate fraction, and (7) a corrosivity assessment of each distillate fraction.<sup>5–7</sup> It has been used to characterize *n*-alkanes,<sup>8</sup> simple azeotropes,<sup>9</sup> gas turbine fuels,<sup>10–15</sup> diesel and biodiesel fuels,<sup>16–21</sup> gasolines,<sup>22–24</sup> rocket propellants,<sup>10,25–28</sup> and crude oils.<sup>29–32</sup> Unlike the conventional distillation curve, fuel volatility or vapor–liquid equilibrium data, ADC data can be modeled with an equation of state.<sup>33–38</sup> Applying the ADC method to the analysis of heavy fuel oil for the first time will provide the physical and chemical data needed to understand and model combustion processes in marine diesel engines.

## 2. MATERIALS AND METHODS

### 2.1. Intermediate Fuel Oil Sample Characterization.

The physical properties and composition requirements for marine diesel fuel are specified in ISO 8217.<sup>39</sup> Intermediate Fuel Oil (IFO 380) is defined principally as a blend of residual oil and distillate fuel with a kinematic viscosity of 380 mm<sup>2</sup>/s (cSt) at 50 °C and maximum density of 0.991 g/cm<sup>3</sup> at 15 °C.

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Limits on the allowable concentration of vanadium, sodium, aluminum, and silicon were incorporated into the fuel specification once their role in high temperature corrosion of engine components became evident.<sup>2</sup> The maximum sulfur concentration allowed is 4.5% by mass or lower, as stipulated by legal requirements where the vessel is operating.

A sample of IFO 380 was obtained from a ship berthed in the Port of Long Beach, California.<sup>40</sup> Pycnometry performed on the sample showed its density to be 0.9867 g/cm<sup>3</sup>, with a combined uncertainty of 0.0006 g/cm<sup>3</sup> under ambient conditions (24.9 °C, 830.8 mbar). Because the density is derived from the measured volume of the container and the mass of the sample, the uncertainty estimates of the two measured values were combined in quadrature to determine the uncertainty of the density. All of the uncertainties reported in this work are estimates of a combined expanded uncertainty with a coverage factor of 2 (i.e., 2 $\sigma$ ).

A commercial rotating cylinder viscometer (inner spindle diameter 1.885 cm, outer boundary diameter 3.200 cm) was used to measure the kinematic viscosity of the sample. The mean kinematic viscosity was measured to be 387 mm<sup>2</sup>/s (cSt) at 50.0 °C and 830 mbar, with an uncertainty of 26 mm<sup>2</sup>/s (cSt) based on five steady-state measurements at two rotational frequencies (6 and 12 rpm).

Wet-ashing of the sample was performed to determine its mineral content and composition. The sample was first charred with concentrated sulfuric acid and then ashed at 540 °C for 6–12 h in a quartz beaker.<sup>41</sup> The mean ash content of three replicate measurements was 0.083% by mass, with a combined expanded uncertainty of 0.010%. X-ray energy dispersive spectroscopy of the ash showed vanadium, nickel, iron, sodium, aluminum, and trace quantities of potassium to be present in the sample.

The asphaltene content of the IFO 380 marine diesel fuel was determined by use of a modified ASTM D6560 test method.<sup>42</sup> A sample of the fuel was placed in a grade 2 (8  $\mu$ m) filter paper cone and refluxed with 10 mL of hexane for 1 h at 100 °C to extract its aliphatic and resinous fractions. The hexane-insoluble asphaltene fraction was then extracted from the filter paper with 10 mL of toluene under reflux for 2 h at 190 °C. The asphaltene content of the sample was determined to be 19.71% (mass/mass) based on three replicate measurements, with a combined expanded uncertainty of 5.50% (mass/mass).

All elements detected in the sample appear to be below the limits specified by ISO 8217. The measured physical and chemical properties of the sample, summarized in Table 1, are typical of IFO 380 marine diesel fuel.

**2.2. Advanced Distillation Curve Method.** The low volatility and high boiling temperature of IFO 380 marine diesel fuel require the sample to be distilled under reduced pressure to avoid thermal degradation, cracking, or polymerization. The reduced-pressure ADC apparatus and sampling method have been described in detail in earlier works, with applications reported for biodiesel fuels,<sup>43,44</sup> crude oils, and waste oils.<sup>45</sup> A limited description of the particular steps employed in this study is provided here.

The boiling flask (kettle) was filled with approximately 100 mL of IFO 380 marine diesel fuel from a beaker. The flask was then weighed on a triple-beam balance to determine the fuel mass. The fuel mass and density at ambient conditions were used to determine its volume. Two thermocouples were inserted into the distillation head and boiling flask to monitor

**Table 1. Specifications and Measured Properties of IFO 380 Marine Diesel Fuel<sup>a</sup>**

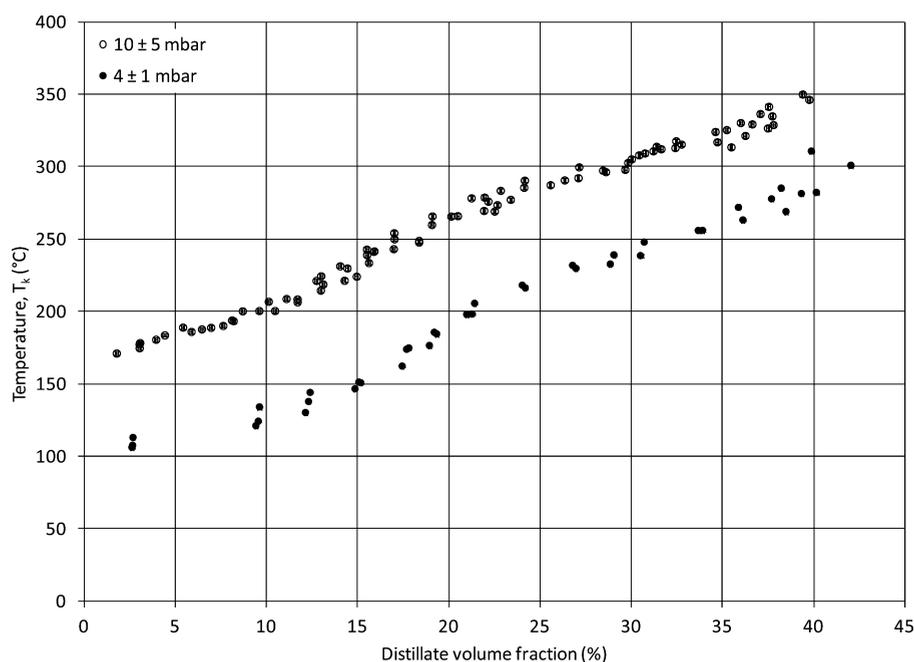
		limit (ISO-F-RMG 380)	measurement	uncertainty
kinematic viscosity		380.0 mm <sup>2</sup> /s (at 50 °C)	387 mm <sup>2</sup> /s (at 50.0 °C)	13 mm <sup>2</sup> /s
density		991.0 kg/m <sup>3</sup> (at 15 °C)	986.7 kg/m <sup>3</sup> (at 24.9 °C)	0.3 kg/m <sup>3</sup>
sulfur		4.5% (mass/mass)	4.40% (mass/mass)	2.09%
ash		0.100% (mass/mass)	0.083% (mass/mass)	0.010%
trace elements	V	350 mg/kg	284 mg/kg	46 mg/kg
	Na	100 mg/kg	45 mg/kg	21 mg/kg
	Al + Si	60 mg/kg	37 mg/kg	33 mg/kg
	Ca	30 mg/kg	not detected	not applicable
	Zn	15 mg/kg	not detected	not applicable
	P	15 mg/kg	not detected	not applicable
	Ni		110 mg/kg	13 mg/kg
	Fe		36 mg/kg	6 mg/kg
asphaltene			19.71% (mass/mass)	2.75%

<sup>a</sup>Limits are maximum allowable values. See text for discussion of uncertainty in measurement results.

the vapor temperature at the bottom of the distillate takeoff position ( $T_h$ ) and the liquid temperature in the kettle ( $T_k$ ). An aluminum heating enclosure was used to uniformly control the temperature of the fluid. The temperature was increased slowly under manual control to maintain uniform sample heating, using prior distillation data as a guide for the ramp rate.

A commercial proportional, integral, derivative (PID) vacuum controller was connected to the sampling adapter vacuum port to measure and control the system pressure. The pressure transducer was calibrated by measuring the vapor pressure of deionized water as a function of temperature (see the Supporting Information for additional details). The system was purged of oxygen by lowering the system pressure to 4 mbar (400 Pa) and then backfilling to ambient atmospheric pressure with carbon dioxide gas. A gas reservoir containing 1 L of carbon dioxide was connected directly to the vacuum controller as a safety measure. The volume of the carbon dioxide gas in the reservoir exceeds the total system volume of the ADC apparatus. If the system must be brought to atmospheric pressure quickly, the carbon dioxide from the reservoir prevents air from coming into contact with the potentially combustible fluid in the boiling flask and receiver. During earlier trials, a small quantity of air introduced during reduced-pressure sampling caused a smoky white vapor to form in the sampling neck near the adapter hammock. Backfilling the system with carbon dioxide gas prior to the start of the distillation prevents the formation of the smoky vapor during reduced-pressure sampling.

Distillate volume measurements were made in a calibrated volume graduated receiver. The volume calibration was accomplished by adding ink-laced methanol with a volumetric pipet to the receiver. As noted above, the viscosity and opacity of the IFO 380 marine diesel fuel precluded the use of a volumetric pipet to measure and transfer the fuel directly from the storage container to the boiling flask. The sample mass and density at ambient conditions were then used to calculate the



**Figure 1.** Distillation curve data for IFO 380 marine diesel fuel at 4 mbar (with an uncertainty of 1 mbar) and 10 mbar (with an uncertainty of 5 mbar). Here, the temperature of the liquid in the boiling flask (kettle) is plotted as a function of distillate volume fraction. The error bars based on the expanded uncertainties in the measurement are smaller than the plotting symbols in the figure.

**Table 2. Representative Distillation Curve Data for IFO 380 Marine Diesel Fuel at 4 mbar (400 Pa) and 10 mbar (1000 Pa) Given As the Average of Three Replicate Distillations<sup>a</sup>**

pressure, 4 mbar (with uncertainty of 1 mbar)				pressure, 10 mbar (with uncertainty of 5 mbar)			
volume fraction, % (v/v)	$U_c(V)$ , % (v/v)	$T_k$ , °C	$U(T)$ , °C	volume fraction, % (v/v)	$U_c(V)$ , % (v/v)	$T_k$ , °C	$U(T)$ , °C
2.9	0.2	108.9	14.4	3.0	0.0	177.0	3.7
7.8	0.3	122.7	8.9	8.3	0.6	196.0	7.6
9.9	1.1	134.0	15.3	10.0	0.9	202.7	7.4
12.5	0.5	147.3	14.5	12.9	0.4	218.3	6.8
15.0	0.7	162.3	46.2	14.5	0.9	228.6	7.6
16.9	3.3	179.0	23.3	17.0	0.1	246.7	9.6
18.7	2.2	193.6	31.4	19.1	0.0	263.0	8.3
21.3	0.8	221.2	69.7	22.0	0.2	274.9	9.4
24.1	0.8	233.2	70.6	24.1	0.1	288.2	6.9
26.4	2.0	240.4	63.9	25.9	1.1	289.2	4.7
28.3	2.7	248.2	65.4	27.1	0.1	296.1	10.6
31.1	1.6	259.8	56.8	31.4	0.4	312.4	3.1
33.9	0.1	264.0	45.0	32.5	0.4	315.5	4.7
36.2	1.0	275.4	44.8	35.6	0.8	323.2	17.3
38.2	1.6	287.0	85.7	37.5	0.1	334.2	21.1
40.4	1.5	291.6	52.9	39.6	0.5	348.3	5.2

<sup>a</sup>Combined expanded uncertainty ( $U_c$ ) values with a coverage factor of 2 are shown to the right of their respective measured values.

initial volume. The uncertainty estimates of the three measured values (fuel mass, density, and distillate volume) were combined in quadrature to determine the uncertainty of the distillate volume fraction.

**2.3. Gas Chromatography with Flame-Ionization Detection (GC-FID).** Sample aliquots of distillate cuts were collected with a pressure-balance syringe at the adapter hammock and dissolved in *n*-hexane inside a sealed autosampler vial.<sup>43,44</sup> Due to the high asphaltene content of this IFO 380 marine diesel fuel sample, the choice of *n*-hexane as a solvent greatly reduced the likelihood of introducing asphaltenes into the gas chromatography column. The *n*-hexane solvent used was purchased from a commercial supplier and

determined to be approximately 99% (mass/mass) pure through gas chromatography with flame-ionization detection (stabilized equivalent of 5% phenyl/95% dimethylpolysiloxane column, 30 m × 0.25 mm, nitrogen carrier gas at 207 kPa or 30.0 psi inlet pressure, temperature program from 50 to 400 °C at a heating rate of 5 °C/min).<sup>46</sup> The solvent was used without further purification. Up to ten aliquots were withdrawn at predetermined distillate volume fractions for composition analysis. The diluted fuel aliquots were evaluated GC-FID, as described earlier.

**2.4. Sulfur Chemiluminescence Detection (SCD).** Aliquots of distillate fractions or cuts were collected with a pressure-balance syringe at the adapter hammock and added to

autosampler vials containing toluene. The postdistillation residue in the flask was sampled with a Pasteur pipet and also dissolved in toluene for analysis. Toluene was used instead of *n*-hexane to maximize the solubility of asphaltenes, since the sulfur content of the asphaltene fraction is a significant fraction of the total sulfur present in the sample. The sulfur content of each aliquot was analyzed on a commercially available gas chromatograph equipped with a sulfur chemiluminescence detector (GC-SCD), with the GC inlet connected to the detector with a short retention gap instead of a gas chromatography column (fused silica capillary, 1 m  $\times$  0.25 mm, nitrogen carrier gas at 41.4 kPa or 6.0 psi inlet pressure, split ratio of 0.5:1, column temperature at 200 °C, and detector temperature at 250 °C). A background correction was performed with toluene; the small, nonzero response of the sulfur chemiluminescence detector to toluene was subtracted from each of the sample values to obtain the corrected sulfur signal. The total sulfur concentration in each vial was determined with a calibration curve prepared with solutions of dimethyl sulfoxide dissolved in toluene.

### 3. RESULTS AND DISCUSSION

**3.1. Distillation Behavior.** The distillation curve data are shown graphically in Figure 1 and summarized in Table 2. For the ADC method, we typically record the temperatures at which we visually observe the (a) onset of bubbling, (b) sustained bubbling, and (c) temperature at which vapor is observed to rise into the distillation head. The onset of bubbling and sustained bubbling temperatures are useful as diagnostics during distillation. The vapor rise temperature is the theoretically significant initial boiling temperature (IBT) of the complex fluid. This temperature is important because the composition of the fluid in the boiling flask is known at the start of the distillation. The measured IBT values are provided in Table 3. An increase in the initial boiling temperature of 34 °C

**Table 3. Vapor Rise or Initial Boiling Temperature (IBT) for IFO 380 Marine Diesel Fuel Based on the Average of Three Replicate Distillations**

pressure, mbar	U(P), mbar	IBT, °C	U(T), °C
4	1	90.7	6.8
10	5	124.6	13.4

is observed when the pressure is increased from 4 mbar (with an expanded uncertainty of 1 mbar) to 10 mbar (with an expanded uncertainty of 5 mbar). In general, decreasing the pressure shifts the temperatures of the distillation curve to lower values without changing its shape. The distillation behavior of IFO 380 is consistent with this general principle, as seen in Figure 1.

The shape of the distillation curve can provide information about the composition of the heavy fuel oil. The distillation curve of a complex fluid often contains one or more inflection points as a function of the initial fluid composition. We note some inflections in the distillation curve of IFO 380 marine diesel fuel. An inflection point in the distillation curve is observed around 19% (v/v), at a temperature of 210 °C, for distillations performed at 4 mbar; a similar inflection is seen around 17% (v/v), at a temperature of 245 °C, when the pressure is increased to 10 mbar. Since IFO 380 marine diesel fuel is a blend of residual and marine gas oil, the inflection point likely reflects the change in the distillate composition as it

becomes enriched in heavier hydrocarbon molecules from the residual oil and depleted of the lighter gas oil content. Additional evidence for this transition may be found by examining the distillate composition as a function of distillate volume fraction.

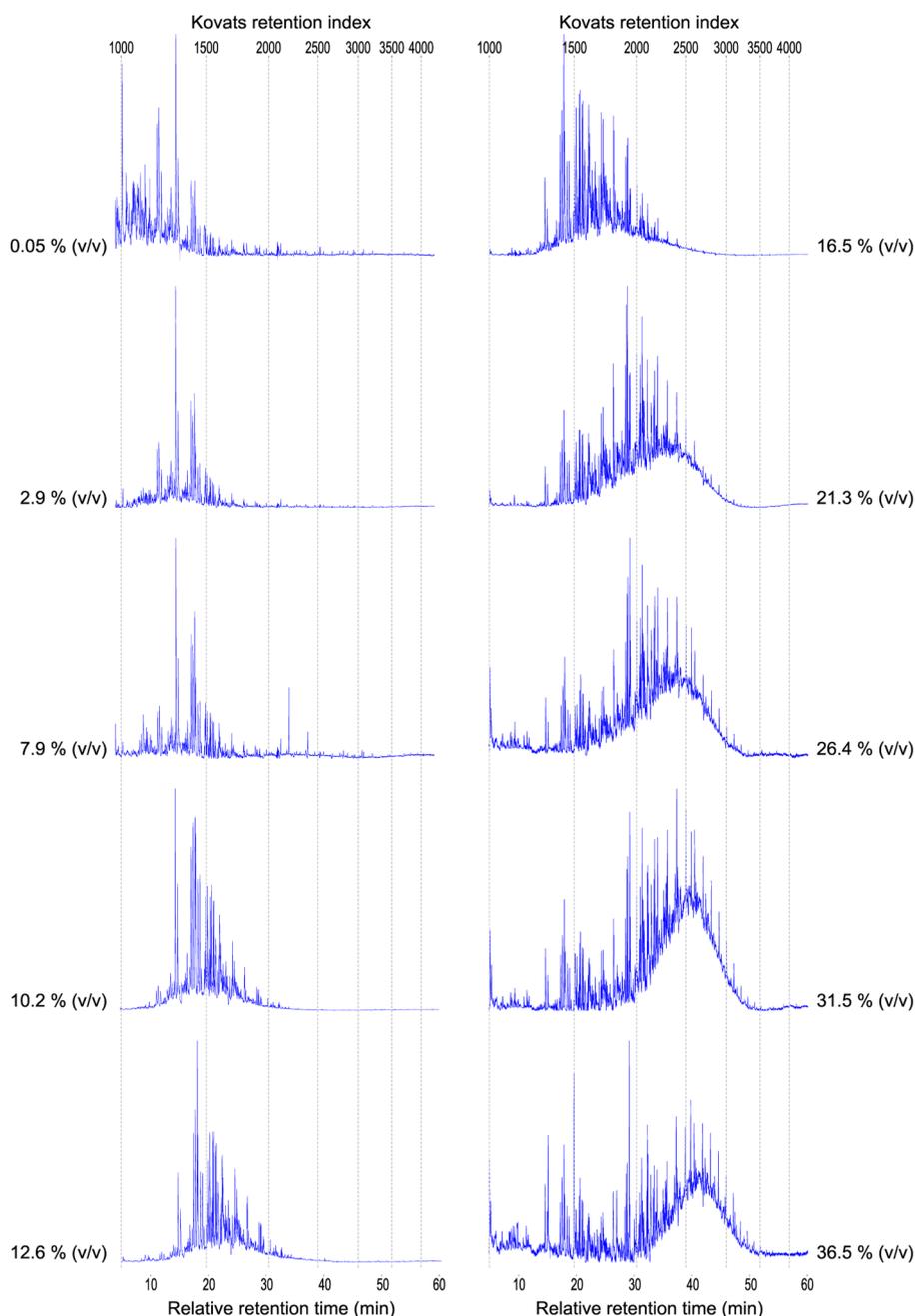
The distillation was stopped at 350 °C to minimize the effect of hydrocarbon cracking and to maintain a margin of safety for working with borosilicate glass under reduced pressure. Approximately 56% (v/v) of the marine diesel fuel remained in the boiling flask at the end of each measurement, as determined through pycnometry and residue mass. Up to 2 mL of condensate was recovered from the cold trap at the end of each distillation. The viscosity and density (1.017 g/cm<sup>3</sup> with an expanded uncertainty of 0.022 g/cm<sup>3</sup>) of the tar-like residue were both greater than the starting material. No further physical or chemical analysis was performed on the residue.

**3.2. Distillate Composition.** While the general shape of the distillation curves is instructive and suffices for many purposes, the composition channel of the ADC method provides more detailed information useful in understanding the thermophysical and chemical properties of complex fluids. Sample chromatograms as a function of distillate volume fraction are shown in Figure 2 and are representative of the data collected through the composition channel during each distillation. The flame-ionization detector response has been normalized to the maximum peak height for each chromatogram. Due to the use of *n*-hexane as the solvent, asphaltene molecules present in the distillate are expected to precipitate and should not contribute to the resultant chromatogram. Trace contaminant peaks from the *n*-hexane solvent and column-induced artifacts (baseline drift and polysiloxane peaks) were removed digitally during data analysis (see the Supporting Information for additional details).

The Kovats retention index (I) is a commonly used metric for reporting analyte retention periods relative to *n*-alkane standards for a given stationary phase.<sup>47</sup> The index assigns a value of 100 times the carbon number of each *n*-alkane (e.g., I = 600 for hexane, 700 for heptane, etc.). The retention periods for *n*-alkanes with carbon numbers 10 to 30 on the thermally stabilized 5% phenyl/95% dimethylpolysiloxane-equivalent column were measured using the same temperature program and used to assist in the characterization of peaks present in the chromatograms. The Kovats retention indices derived from reference standards are overlaid on the chromatograms in Figure 2.

The development of a broad unresolved complex mixture (UCM) hump becomes apparent for distillate volumes greater than 10.2% (v/v). The hump contains numerous coeluting components that cannot be resolved by use of the current gas chromatography method, contributing to a bell-like shape described by a normal or Gaussian distribution. Resolved *n*-alkane peaks are also present in the chromatograms and can be found superimposed on top of the UCM hump. The increase in the relative peak height over the tridecane to hexadecane (1300 < I < 1600) range for distillate cuts greater than 26.4% suggests thermal cracking of the heavy hydrocarbons present in the residual oil portion of the IFO 380 marine diesel fuel.

**3.3. Total Sulfur Content.** The sulfur content varies as a function of distillate volume fraction. Table 4 shows the average sulfur concentration from three replicate distillations. The sulfur concentration increases with distillate volume, as seen in Figure 3. The average sulfur concentration of the IFO 380 was found to be 4.40% (mass/mass) through numerical integration,



**Figure 2.** Chromatograms of IFO 380 marine diesel fuel distillate fractions, presented in arbitrary units of intensity (based on flame-ionization detector current output) plotted as a function of time. Kovats retention index values are plotted for reference and are discussed in the text.

with an expanded uncertainty of 2.09% (mass/mass). Sulfur adsorbs readily on glass and metal surfaces, leading to a systematic decrease in the detector response as a function of time. Freshly collected samples must be analyzed with the sulfur chemiluminescence detector immediately after each distillation to minimize the effect of sulfur adsorption on the measured signal. We are investigating the use of an amorphous silicone-coated stainless steel in sample collection and storage to mitigate this effect in the future.

The increase in the sulfur content with distillate volume and large variability in the measured sulfur concentration are explained by the presence of asphaltenes in the residual oil fraction of IFO 380 marine diesel fuel. Asphaltenes contain from 0.3% to 10.3% sulfur by mass. Sulfur is incorporated into the polycyclic aromatic hydrocarbon structure of asphaltenes as

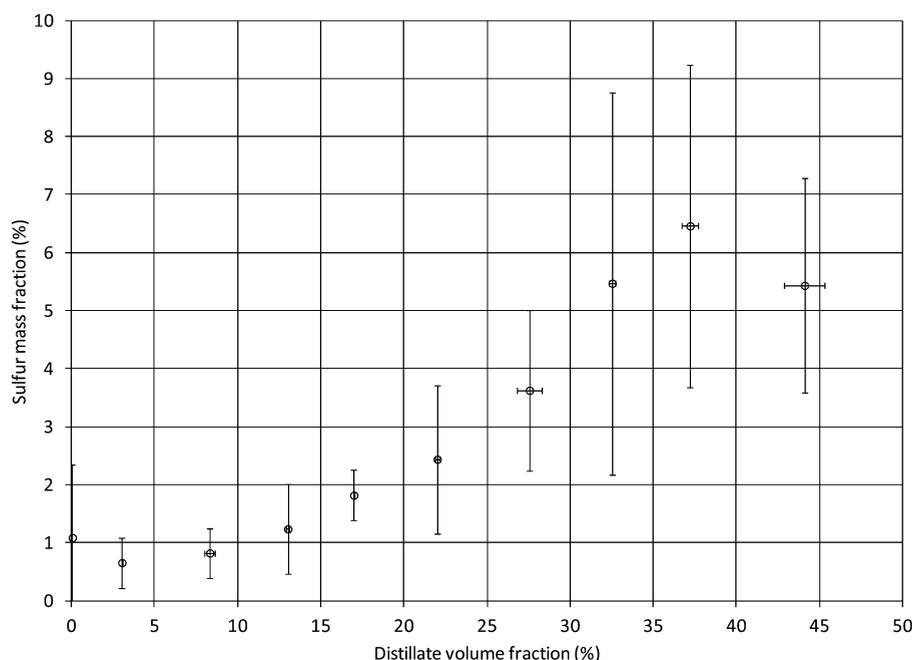
heteroatoms, which are difficult to remove through heating.<sup>48</sup> The increase in viscosity, density, and sulfur concentration suggests that asphaltenes are concentrated in the residue fraction as more volatile components of the IFO 380 are removed through distillation.

Analysis of the neat IFO 380 marine diesel fuel dissolved in toluene using the same protocol underestimates its sulfur concentration: 1.52% (mass/mass) with an expanded uncertainty of 1.03% (mass/mass) based on twenty-two replicate measurements. The high asphaltene content of the fuel provides an explanation for the lower measured sulfur content of the neat IFO 380 marine diesel fuel compared with the value obtained by numerically integrating the sulfur concentrations of the distillate and residual fractions. The difficulty of volatilizing high molecular-weight asphaltenes means that some of the

**Table 4. Sulfur Content of IFO 380 Marine Diesel Fuel As a Function of Distillate Volume Fraction at a Pressure of 10 mbar with an Uncertainty of 5 mbar Measured with GC-SCD<sup>a</sup>**

distillate cut	volume fraction, % (v/v)	$U_c(V)$ , % (v/v)	$T_b$ , °C	$U(T)$ , °C	sulfur concentration, % (mass/mass)	$U_c(m)$ , % (mass/mass)
A (first drop)	0.05		135.0	17.8	1.09	1.27
B	3.03	0.19	177.0	4.0	0.66	0.44
C	8.32	0.66	196.0	7.7	0.82	0.43
D	13.01	0.23	219.4	10.0	1.24	0.77
E	16.98	0.16	249.2	11.2	1.82	0.43
F	22.00	0.28	274.9	9.6	2.44	1.27
G	27.55	1.54	296.5	7.8	3.63	1.39
H	32.53	0.39	315.5	5.0	5.47	3.29
I	37.21	1.03	332.6	15.9	6.46	2.77
J (residue)	>44.10	2.40			5.43	1.85

<sup>a</sup>Combined standard uncertainty ( $U_c$ ) values with a coverage factor of 2 are shown to the right of their respective measured values.

**Figure 3.** Sulfur concentration as a function of distillate volume fraction.

sulfur present in the neat fuel will not reach the detector at the operating temperature of the GC-SCD. By first fractionating and cracking the complex fluid, the composition channel of the ADC method provides a more accurate measurement of the sulfur content within the IFO 380 marine diesel fuel.

#### 4. CONCLUSIONS

In this paper, we applied the ADC method to the analysis of commercial IFO 380 marine diesel fuel and measured its distillation curve at two pressures. Since the initial boiling temperature results are thermodynamic state points, these data are amenable to the development of equations of state for marine diesel fuel. The shape of the distillation curve can be ascribed to the blend of distillate gas oil and residual oil used in the production of marine diesel fuel. Composition analysis by use of gas chromatography with flame ionization detection suggests the thermal cracking of complex hydrocarbons at high temperatures. Sulfur chemiluminescence detection indicates that sulfur concentration is positively correlated with distillate volume fraction. This work is significant in illustrating the applicability of the reduced-pressure ADC approach to the analysis of heavy fuel oils by providing the thermophysical and

chemical data needed to unravel the complex interactions occurring during combustion in a marine diesel engine. The data given in Tables 2, 3, and 4 provide a starting point in the development of an equation-of-state for IFO 380 marine diesel fuel in the future.

#### ■ ASSOCIATED CONTENT

##### Supporting Information

Figures S1–S3, Table S1, and text. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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##### Notes

The authors declare no competing financial interest.

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## ABBREVIATIONS AND ACRONYMS

ADC = Advanced Distillation Curve  
ASTM = ASTM International (formerly American Society for Testing and Materials)  
GC-FID = gas chromatography with flame ionization detection  
GC-SCD = gas chromatography with sulfur chemiluminescence detection  
I = Kovats retention index  
IBT = initial boiling temperature  
IFO = intermediate fuel oil  
ISO = International Organization for Standardization  
NIST = National Institute of Standards and Technology  
PID = proportional, integral, derivative  
T<sub>h</sub> = headspace temperature  
T<sub>k</sub> = kettle temperature  
UCM = unresolved complex mixture

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