PHOTOACOUSTIC INFRARED SPECTROSCOPY AND THERMOPHYSICAL PROPERTIES OF SYNCRUDE COKES

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Abstract

This paper presents and interprets photoacoustic (PA) infrared spectra and four different thermophysical properties (thermal conductivity, thermal diffusivity, volumetric specific heat and thermal effusivity) for four sets of hydrocarbon cokes. A total of 12 samples, with varying histories, were analyzed. These cokes are a by-product of the upgrading of bitumen to Syncrude Sweet Blend (a blend of hydrotreated components), and were obtained from several locations in the thermal cokers operated by Syncrude Canada Ltd. in Fort McMurray, Alberta, Canada.

PA infrared spectroscopy provides detailed information on the amount and type of residual aromatic hydrocarbons in cokes; aliphatic hydrocarbons are sometimes detected in smaller quantities. Three of the thermophysical properties (thermal conductivity, diffusivity and effusivity) display systematic differences among the cokes. On the other hand, volumetric specific heat hardly varies, a phenomenon that accounts for the observed proportionality between thermal diffusivity and conductivity. Analogous relationships exist between thermal effusivity and both thermal conductivity and thermal diffusivity for these cokes. The magnitudes of these three thermophysical properties tend to increase as aromatics contents, determined by PA spectroscopy, decrease.

Keywords: photoacoustic infrared spectroscopy, thermal conductivity, thermal diffusivity, thermal effusivity, thermophisical propertties

Introduction

The Athabasca oil sand deposits in northeastern Alberta contain more than one trillion barrels of bitumen, and are among the largest reserves of hydrocarbons known to exist. The extraction of this bitumen and its subsequent upgrading to Syncrude Sweet Blend (SSB, a blend of hydrotreated components) inevitably lead to the production of large quantities of coke. This carbonaceous solid consists of approximately 90 per cent carbon, 4 per cent sulphur, and residual aromatic hydrocarbons, typically at the

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level of about 1 per cent. Trace (parts per million) amounts of metals such as iron, nickel, vanadium and titanium also occur in this coke.

The high carbon content in cokes makes it particularly difficult to distinguish among them even when they are produced under different conditions or from different feedstocks. For example, Raman spectra of cokes resemble those of many other carbons, clearly displaying the well-known 'D' and 'G' bands [1]; however, these spectra barely differ from one coke to the next. Numerous other chemical and physical techniques also fail to differentiate these cokes. Thus, the present work is motivated by the need to develop analytical methods that satisfactorily characterize cokes, while minimizing any sample preparation that could lead to the modification of either their surface or bulk properties.

Photoacoustic (PA) infrared spectroscopy is a well-established technique that has been used successfully in recent years to characterize solids such as coals [2, 3], clays and clay complexes [4, 5], as well as a variety of problematic or unusual samples. In a typical gas-microphone cell, the PA effect involves several steps: (a) infrared radiation absorbed within the sample is converted into heat; (b) this heat propagates to the cooler surface of the sample; (c) the sample radiates heat to the carrier gas in the cell; and (d) a microphone detects the resulting pressure (acoustic) wave in the gas. PA detection of infrared spectra offers several advantages that are relevant in the present context; most importantly, the technique requires virtually no sample preparation, and sampling depth can be controlled. It is evident that both of these features are pertinent to the analysis of heterogeneous samples such as cokes.

The importance of heat transfer in a PA infrared experiment suggests an investigation of the thermophysical properties of the samples under investigation. For example, the PA signal arises from a surface layer having a thickness that is proportional to the square root of thermal diffusivity (α). This quantity is related to thermal conductivity (κ) and volumetric specific heat (ρC_p) by $\alpha = \kappa / \rho C_p$, where ρ and C_p denote density and specific heat, respectively. Moreover, the exchange of heat between the sample and the carrier gas is governed by thermal effusivity (e), which can be regarded as the thermal analogue of electrical impedance. These thermophysical properties were measured (α, κ, e) or calculated (ρC_p) for several sets of Syncrude cokes in this work. PA infrared spectroscopy was also used to study these samples. The results of both analyses show that it is indeed possible to successfully characterize these cokes; infrared spectroscopy proves to be most effective with respect to detection of the hydrocarbon component, whereas the thermophysical properties appear to be determined primarily by the carbon matrix of the cokes.

Experimental

Materials

Four different sets of cokes (a total of 12 samples) were obtained from the Syncrude upgrading plant at Fort McMurray, Alberta for this study. These four groups are referred to as wall, core, 'chunky' and 'shark fin' cokes, respectively (Table 1). The

Table 1 Thermophysical properties of Syncrude cokes[a,b]

Coke	Description	κ/W m^{-1} K^{-1}	α/10^{-6} m^2 s^{-1}	ρC_p/10^6 J m^{-3} K^{-1}	e/W s$^{1/2}$ m^{-2} K^{-1}
A		0.6374 (0.0015)	0.5917 (0.0270)	1.079 (0.050)	1032 (3.6)
B	wall	0.5747 (0.0022)	0.4683 (0.0119)	1.228 (0.027)	985.5 (2.3)
C		0.5868 (0.0017)	0.4699 (0.0125)	1.249 (0.030)	978.5 (2.3)
D		0.5226 (0.0012)	0.4381 (0.0024)	1.193 (0.004)	902.6 (2.2)
E	core	0.4685 (0.0010)	0.4010 (0.0018)	1.169 (0.006)	897.4 (6.6)
F		0.4552 (0.0012)	0.3961 (0.0133)	1.150 (0.037)	865.5 (1.1)
G	chunky	0.5956 (0.0024)	0.4290 (0.0034)	1.394 (0.006)	1009 (33.5)
H		0.9126 (0.0018)	0.6175 (0.0019)	1.478 (0.004)	1224 (8.3)
I		0.4896 (0.0270)			883.7 (64.0)
J	shark fin	0.5361 (0.0121)			961.0 (18.2)
K		0.5162 (0.0081)			938.5 (3.9)
L		0.5410 (0.0142)			975.0 (5.8)

[a]Definitions of symbols for thermophysical properties: κ – thermal conductivity; α – thermal diffusivity; ρC_p – volumetric specific heat; e – thermal effusivity. ρC_p was calculated using the relation $\alpha = \kappa/\rho C_p$ (see text).
[b]Values in parentheses represent one standard deviation.

wall and core cokes formed on the walls of a large (10×30 m) fluidized-bed thermal coking unit in the plant; the pieces of wall coke were of random size and shape, while the 45 mm diameter wall coke core was cut into sections having a thickness of about 12 mm. The chunky cokes are formed by condensation of fluid coke particles that circulate in the coker. Shark fin cokes, which take their name from their characteristic shape, are formed on internal structures near the centre of the coker.

Methods

PA infrared spectra were recorded at a resolution of 8 cm^{-1} using a Bruker IFS 113v Fourier Transform Infrared (FT-IR) spectrometer and a Princeton Applied Research Corporation model 6003 PA cell. The use of this apparatus is straightforward and has been described previously [3, 4]. A few milligrams of each coke was scraped or chipped from the original larger (40–100 mm) pieces, and analyzed without further preparation. Several (2–5) subsamples of each coke were analyzed by infrared spectroscopy. The PA spectra of the cokes were corrected for frequency-dependent instrumental effects through division by spectra of carbon black powder obtained under similar conditions.

The thermophysical data in this paper were obtained with two different pieces of equipment. A Hot Disk™ Thermal Constants Analyser (Hot Disk Inc., Uppsala, Sweden) was used to measure thermal conductivity and thermal diffusivity for the wall cokes, core samples and chunky cokes. This apparatus was located in the applications laboratory of Mathis Instruments Ltd., Fredericton, New Brunswick, Canada. It employs transient interfacial heating to determine κ and α, from which ρC_p can be calculated (see above). Thermal effusivities of all 12 cokes, in addition to the thermal conductivities of the four shark fin cokes, were obtained using a TC Probe™, which employs transient interfacial heat reflectance in a modified hot-wire technique and is manufactured by Mathis Instruments Ltd. This instrument is installed at CANMET Western Research Centre in Devon, Alberta, Canada. Before testing, the cokes were sawn to produce flat faces with lateral dimensions of at least 40 mm, permitting good thermal contact with both types of apparatus.

Results

PA infrared spectra

Representative infrared spectra of the four types of Syncrude cokes are presented in this section. The examples are chosen so as to illustrate the most important trends in the PA infrared spectra of all 12 cokes. Figures 1a and 1b depict spectra of core (F) and chunky (G) cokes, while typical results for wall and shark fin cokes are shown in Figs 1c and 1d, respectively.

There are a number of important features in the spectrum of core coke F (Fig. 1a). For example, in the region between 700 and 900 cm^{-1} three prominent bands are observed at 750, 810 and 870 cm^{-1}. These bands arise from out-of-plane vi-
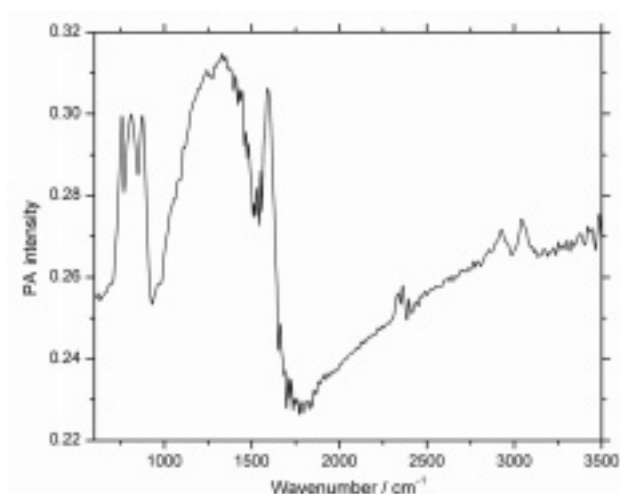
Fig. 1a PA infrared spectra of core coke F
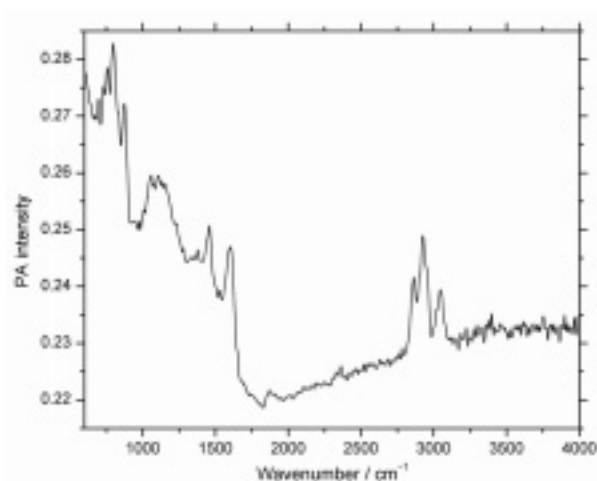
Fig. 1b PA infrared spectra of chunky coke G

brations of aryl C–H groups in substituted aromatic rings, and are analogous to those observed in infrared spectra of model aromatic compounds and some high-rank coals. Their intensities indicate a comparatively high concentration of aromatic hydrocarbons in this coke. The assignments of these bands are well known; in general, frequency decreases as the number of contiguous hydrogens participating in the vibration increases. Specifically, the 870 cm^{-1} band is assigned to isolated C–H groups, while the broader 810 cm^{-1} peak arises from species containing two or three adjacent hydrogens, and the 750 cm^{-1} band indicates the presence of an aromatic ring with four neighbouring H atoms. To a first approximation, the comparable intensities exhibited by these bands imply similar concentrations of these three species in coke F.
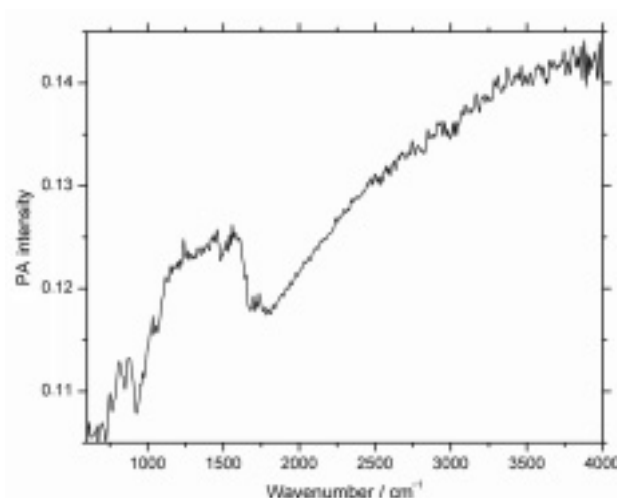
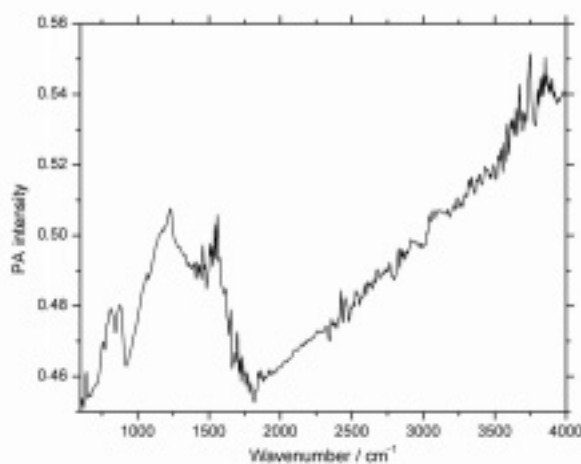**Fig. 1c** PA infrared spectra of wall coke D

Fig. 1d PA infrared spectra of shark fin coke K

Near the high-frequency end of the fingerprint region, the strong 1600 cm^{-1} band is due to aromatic C=C stretching, and is analogous to the bands observed at this frequency in infrared spectra of various carbons and medium-temperature chars [6]. At still higher frequencies, bands due to aliphatic (2925 cm^{-1}) and aromatic (3050 cm^{-1}) C–H stretching are observed. The predominantly aromatic nature of the residual hydrocarbon in coke F is confirmed by the fact that the aromatic C–H band is the stronger of the two in this region. These results for the C–H stretching bands are particularly noteworthy when it is recalled that aliphatic C–H intensity generally exceeds ar-

omatic intensity by a factor of 30 or more in PA spectra of bitumens and distillation fractions derived from SSB [7].

Another indication of the aromatics content in coke F is the continuum in the region between 1800 and 3500 cm^{-1}, which intensifies with increasing wavenumber. This very broad feature arises from low-energy electronic absorption in aromatic hydrocarbons, and is also observed in the PA spectra of high-rank coals, where it extends to near-infrared [3] and visible wavelengths. Its presence in Fig. 1a is consistent with the other features attributed to aromatics in the previous two paragraphs.

The PA infrared spectrum of coke G (Fig. 1b) is qualitatively different from that of coke F (Fig. 1a). In fact, bands due to aliphatic species are quite prominent in the spectrum of the chunky coke: in Fig. 1b, CH_2 and CH_3 deformation and wagging vibrations give rise to peaks at 1377 and 1458 cm^{-1}, while the aliphatic C–H stretching region displays bands at 2865 and 2928 cm^{-1}, as well as a shoulder at 2955 cm^{-1}. This spectrum also displays most of the bands due to aromatics that were discussed above, although the continuum above 1800 cm^{-1} is less intense in Fig. 1b. In summary, the PA infrared spectrum of this chunky coke shows that it contains measurable quantities of both aliphatic and aromatic hydrocarbons, the aliphatic component being the more abundant of the two.

Figure 1c depicts the PA infrared spectrum of wall coke D. This spectrum exhibits obvious similarities with the result for coke F (Fig. 1a). In particular, the three aromatic C–H bands between 700 and 900 cm^{-1} discussed earlier are also observed for coke D. Although Fig. 1c displays a rather poorly defined 1600 cm^{-1} band, there is a fairly intense absorption continuum that extends toward the near-infrared. Hence the presence of aromatic hydrocarbons in coke D is confirmed by its PA spectrum; comparison with Fig. 1a implies that coke D possesses somewhat lower aromatics content. Moreover, it can be noted that the 750 cm^{-1} aromatic C–H band is weaker than its two counterparts in Fig. 1c, in contrast with the result for the core sample. This suggests that coke D contains aromatics with a substitution pattern different from that for coke F.

The infrared spectrum of coke K is presented in Fig. 1d. This result is similar to that in Fig. 1c in several respects, leading to the conclusion that the aromatic hydrocarbons present in coke K are similar in nature and concentration to those in coke D. However, Fig. 1d contains one feature that has not been identified or discussed previously: a band at 1225 cm^{-1} is superimposed on the broad, nearly featureless absorption that most of the coke spectra exhibit between about 900 and 1500 cm^{-1}. There is no likely assignment involving a hydrocarbon functional group at this frequency. On the other hand, as mentioned in the introduction, these cokes are known to contain sulphur at concentrations as high as four per cent; this suggests the attribution of the 1225 cm^{-1} band to a sulphur-bearing group. Accordingly, this band is tentatively assigned to C=S stretching or CH_2S deformation [8], which could occur in compounds such as thiols, sulphides or disulphides. Confirmation of this assignment may eventually require the use of other techniques, such as X-ray absorption spectroscopy.

Thermophysical properties

The values measured for thermal diffusivity, conductivity and effusivity, as well as those calculated for volumetric specific heat, are listed in Table 1. As noted in the experimental section, a Hot Disk™ instrument was utilized to determine 6 for cokes A–H, while a TC Probe was used to measure this property for the shark fin cokes. The former instrument also yielded data for, enabling the calculation of ρC_{p}. On the other hand, was not measured with the TC Probe; consequently, volumetric specific heats are not available for cokes I–L.

The standard deviations observed in the thermophysical properties are shown in parentheses in Table 1, and provide an indication of the possible error in each result. It should be noted that some of the larger variations, such as those observed for the thermal effusivities of cokes G and I, probably arise from sample heterogeneity and the fact that relatively small (25 mm) regions of the sample were tested in each of several experiments performed on these cokes. By contrast, the smaller deviations observed for many of the other samples suggest that they possess a greater degree of homogeneity. The latter results also confirm that the intrinsic uncertainties in the transient interfacial measurements – which are based on comparisons between the cokes and standards with known thermal properties – are generally small (typically less than five per cent).

Table 1 shows that three of the thermophysical properties (κ, α and e) differ significantly for cokes A–L. On the other hand, the volumetric specific heats determined for cokes A–H hardly differ, displaying an average value of $1.24\pm0.13\cdot10^{6}$ J m^{-3} K^{-1}. As stated in the introduction, the identification of experimental techniques that characterize and distinguish cokes is a general objective of this research; the data in this table suggest that the above three thermophysical properties differ sufficiently that they can be employed to accomplish this task.

From their definitions, it is apparent that the thermophysical properties are not completely independent of each other. As noted above, volumetric specific heat is equal to the ratio of κ to α. Moreover, e is linked to volumetric specific heat and thermal conductivity via $e=[\rho C_{p}\kappa]^{1/2}$. These relationships suggest that several correlations may exist among the thermophysical properties in Table 1. This prediction is confirmed by the results presented in the following paragraphs.

As mentioned earlier, the volumetric specific heat for these cokes is approximately equal to $1.24\cdot10^{6}$ J m^{-3} K^{-1}. If this value for ρC_{p} is substituted in the relationship between α and κ, one obtains

$$\alpha\approx\kappa/1.24\cdot10^{6} \text{ J m}^{-3} \text{ K}^{-1}$$
$$\alpha\approx(0.805\cdot10^{-6} \text{ J}^{-1} \text{ m}^{3} \text{ K})\kappa \tag{1}$$

In other words, thermal diffusivity should be approximately proportional to thermal conductivity for Syncrude cokes.

The relationship between α and κ for cokes A–H is shown in Fig. 2. As expected, the plotted data exhibit a systematic increase in α as κ increases. This trend holds for three different types of coke, for which κ varies by a factor of about two.

The straight line shown in Fig. 2 is a plot of Eq. (1); the experimental results are observed to agree satisfactorily with the prediction. Thus, the near proportionality between α and κ for these cokes is confirmed to exist. It can be noted that the data for the chunky cokes (plotted as open circles) and for coke A (filled square near the centre of the graph) are farthest from this line, which is to be expected because the volumetric specific heats of these three cokes are significantly different from the average value of $1.24 \cdot 10^6$ J m^{-3} K^{-1} (Table 1).
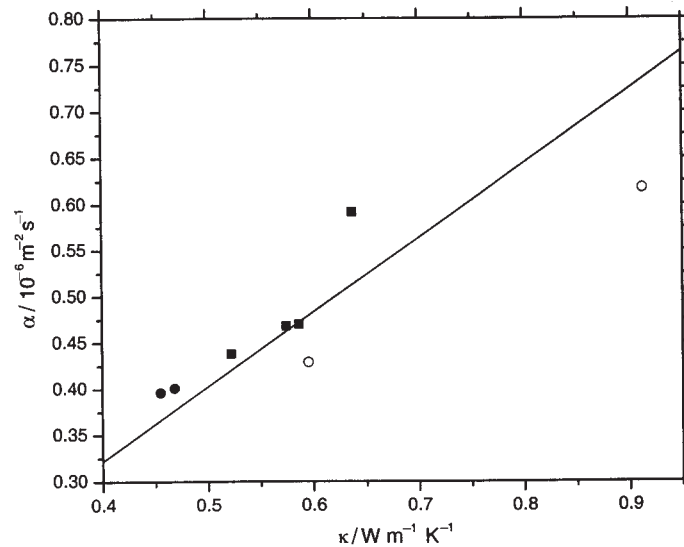

Fig. 2 Variation of thermal diffusivity (α) with thermal conductivity (κ) for Syncrude cokes. Filled circles, core cokes; open circles, chunky cokes; filled squares, wall cokes. The straight line is a plot of Eq. 1, and corresponds to the average value $1.24 \cdot 10^6$ J m^{-3} K^{-1} for the volumetric specific heat

The other two correlations of interest involve thermal effusivity and either of two other thermophysical properties, thermal conductivity or thermal diffusivity. In general, the relationship between e and κ is not straightforward because it also involves ρ and C_p. However, this work has empirically shown the approximate constancy of the volumetric specific heat, ρC_p. If the average value given above for this quantity is substituted into the definition for e, one obtains

$$e \approx [(1.24 \cdot 10^6 \text{ J m}^{-3} \text{ K}^{-1})\, \kappa]^{1/2}$$

$$e \approx (1.11 \cdot 10^3 \text{ J}^{1/2} \text{ m}^{-3/2} \text{ K}^{-1/2})\, \kappa^{1/2} \tag{2}$$

Therefore, e should be approximately proportional to the square root of κ for Syncrude cokes. Similarly, the near proportionality between α and κ demonstrated in Eq. (1) and Fig. 2 implies that e should vary with α according to

$$e \approx (1.24 \cdot 10^6 \text{ J m}^{-3} \text{ K}^{-1})\, \alpha^{1/2} \qquad (3)$$

This reasoning can be evaluated by examining Figs 3 and 4. Figure 3 illustrates the relationship between thermal effusivity and thermal conductivity; error bars are used to represent the standard deviations in e (Table 1) that are larger than the plotted symbols for the various cokes. Indeed, e is roughly proportional to $\kappa^{1/2}$ as suggested by Eq. (2) The slope of the line fitted to the experimental points for all 12 cokes is $1.31 \cdot 10^3$ J$^{1/2}$ m$^{-3/2}$ K$^{-1/2}$, about 18 per cent higher than that predicted in Eq. (2) Similarly, Fig. 4 depicts the dependence of thermal effusivity on diffusivity. Although the data (particularly for chunky cokes) are somewhat scattered, a linear fit of the points in this graph yields a slope of $1.59 \cdot 10^6$ J m^{-3} K^{-1}. This result is noticeably higher than the value predicted in Eq. (3) However, it is relevant to point out that omission of the data for the chunky cokes (plotted as open circles in Fig. 4) produces a slope of $1.16 \cdot 10^6$ J m^{-3} K^{-1}, in good agreement with Eq. 3. As discussed earlier, the chunky cokes are formed in a process different from that for the wall cokes, so it is not surprising that the thermophysical properties of the two types of cokes differ in some aspects. Hence these analyses confirm the existence of relatively simple relationships between thermal effusivity and either thermal conductivity or thermal diffusivity for Syncrude cokes. These observations are particularly significant, inasmuch as only one of these thermophysical properties need be measured in order to predict the other two with acceptable accuracy.
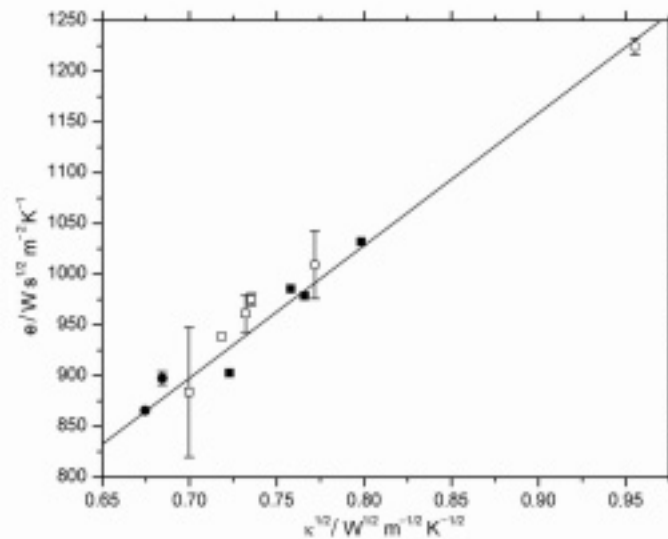

Fig. 3 Dependence of thermal effusivity (e) on thermal conductivity (κ) for Syncrude cokes. Filled circles, core cokes; open circles, chunky cokes; filled squares, wall cokes; open squares, shark fin cokes. The straight line is a least-squares fit, weighted according to the estimated errors in the data

Discussion

Relationship between PA spectra and thermophysical properties

The results presented above confirm that PA infrared spectroscopy is capable of analyzing the residual aromatic and aliphatic hydrocarbons that are present in Syncrude cokes. As mentioned previously, these hydrocarbons occur at concentrations on the order of one per cent; PA spectroscopy enables the non-destructive analysis of this relatively minor component in the presence of a much higher proportion of carbon. The thermophysical properties, on the other hand, characterize the entire coke sample, and can be assumed to be influenced primarily by its carbonaceous nature.
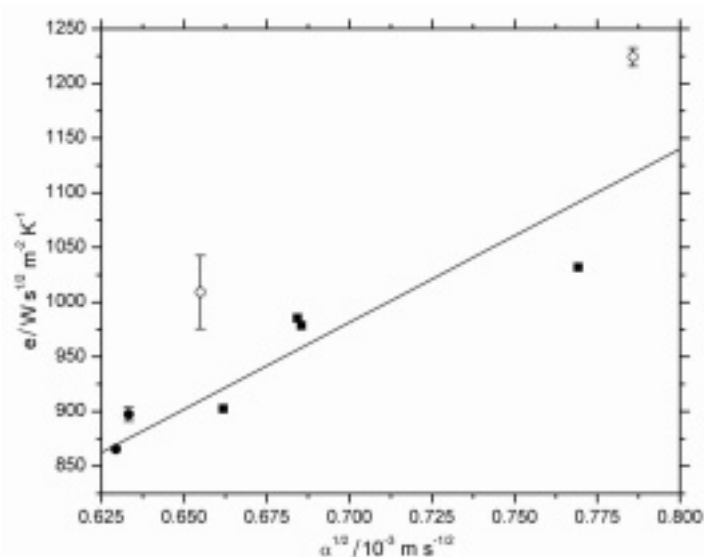

Fig. 4 Variation of thermal effusivity (*e*) with thermal diffusivity (α) for Syncrude
cokes. Filled circles, core cokes; open circles, chunky cokes; filled squares, wall
cokes. The straight line is a least-squares fit, weighted according to the esti-
mated errors in the data

While these two experiments essentially analyze different components of the same sample, the possible existence of a functional relationship between the PA results and the thermophysical data must also be considered. Indeed, a link between the two experiments might be anticipated in view of the fact that PA spectra depend on both the optical and thermal properties of the sample under study. Therefore, if the hydrocarbons present in the cokes affect their thermophysical properties, a distinct relationship between the two experiments can be anticipated.

Comparison of the thermophysical data (Table 1 and Figs 2–4) with the PA infrared spectra (Figs 1a–d) reveals an interesting trend. Table 1 shows that thermal conductivity, thermal diffusivity and thermal effusivity exhibit their smallest values

for the core samples (cokes E and F). As illustrated in Fig. 1a, coke F has the highest aromatic hydrocarbon content of any of the samples studied. On the other hand, coke A possesses very low aromatic hydrocarbon content, whereas cokes B–D exhibit intermediate amounts of aromatics (Fig. 1c). The numerical values of the thermophysical properties of these cokes are all higher than those of the core cokes, with the data for coke A being the highest among the wall cokes (Table 1). This empirical analysis implies that an inverse relationship exists between the magnitudes of the thermophysical properties and the aromatics contents of the Syncrude cokes. The results for cokes D and K are consistent with this prediction: these samples display similar hydrocarbon contents (Figs. 1c and 1d) and thermophysical data (Table 1 and Fig. 3). Moreover, chunky coke H yielded the highest values for the thermophysical properties (Table 1 and Figs. 2–4), while its PA infrared spectrum showed that its hydrocarbon content was the lowest. Thus, the available data indicate that the thermophysical properties assume higher values in cokes with lower aromatics contents. This observation is consistent with the suggestion that the aromatic hydrocarbons occupy the pore structure of a coke, reducing the efficiency of heat propagation through the sample. Further research, on both aromatic hydrocarbons and additional coke samples, will be required to substantiate this model.

Thermal diffusion lengths in PA infrared spectra of cokes

The measurement of α enables the calculation of the thermal diffusion length (μ_s), defined as the distance over which the amplitude of a thermal wave decays to a value equal to $1/e$ (where $e=2.7183$) of its original magnitude. μ_s is an important thermophysical parameter because it provides an indication of the depth to which thermal wave techniques may be used to characterize a sample; to a reasonable approximation, μ_s is equal to the sampling depth in PA infrared spectroscopy.

Calculation of μ_s is straightforward once α is known. The thermal diffusion length is defined mathematically by

$$\mu_s = (\alpha/\pi f)^{1/2} \tag{4}$$

where f denotes modulation frequency. Table 1 shows that α ranges from 0.3961 to $0.6175 \cdot 10^{-6}$ m^2 s^{-1} for the Syncrude cokes studied in this work. Hence a value of $0.5 \cdot 10^{-6}$ m^2 s^{-1} can be considered typical for the thermal diffusivity of Syncrude cokes. For the Bruker IFS 113v FT-IR spectrometer used to record the PA spectra,

$$f = 4V\nu \tag{5}$$

where V denotes mirror velocity (cm s^{-1}) and ν is infrared frequency (cm^{-1}). Typically, the lowest scan velocity of the instrument is used to record PA spectra; according to the manufacturer's specifications, this setting corresponds to $4V=0.235$ cm s^{-1}. At the low-frequency end of the mid-infrared spectrum, $\nu=400$ cm^{-1} and

$$f = (0.235 \text{ cm s}^{-1}) (400 \text{ cm}^{-1}) = 94 \text{ s}^{-1} \tag{6}$$

Substitution in Eq. (4) yields the thermal diffusion length:

$$\mu_s = (0.5 \cdot 10^{-6} \text{ m}^2 \text{ s}^{-1}/\pi 94 \text{ s}^{-1})^{1/2}$$

$$\mu_s = 41.1 \cdot 10^{-6} \text{ m} = 41.1 \text{ μm} \tag{7}$$

At the upper end of the mid-infrared region, ν=4000 cm^{-1} and μ_s=13.0 μm. Similar calculations can be used to obtain μs at other FT-IR scan velocities. These results also demonstrate the well-known variation of sampling depth with infrared frequency in a PA spectrum obtained with a rapid-scan instrument.

Conclusions

PA infrared spectra and thermophysical properties of a series of 12 Syncrude cokes were studied in detail in this work. Infrared spectroscopy elucidates the nature and quantity of the residual hydrocarbons present in the cokes. Three thermophysical properties (κ, α and e) display systematic differences for the cokes; because the volumetric specific heats of the samples are approximately constant, simple relationships exist among these three properties. The values of κ, α and e were found to increase as the aromatics contents of the cokes decrease.

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