# Appendix A: Estimation of the total in-place oil and gas resources in Carboniferous shales in the Midland Valley of Scotland

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### 1. Aim

The aim of this study is to estimate the P10-P50-P90<sup>1</sup> range of **total gas in-place** and **total oil inplace volumes** for the Limestone Coal Formation, Lower Limestone Formation, West Lothian Oilshale unit and Gullane unit (Carboniferous) across the Midland Valley of Scotland.

This analysis forms an appendix to the main Midland Valley of Scotland report, which provides the detailed geological background to this shale oil and shale gas play. This specific study applies a Monte Carlo simulation to a suite of input parameters, some of which were a product of the geology-based methodology described in the main report, and others which are based on information from published analogues.

The methodology used for the Midland Valley of Scotland study follows that used by Andrews (2013 & 2014) to assess the prospectivity of the Bowland-Hodder shales of central Britain and Jurassic shales of the Weald area.

Two sets of resource estimates are presented; firstly the best technical case of prospective and potentially exploitable shale oil and shale gas using a mining-related depth cut-off. **These are the resource estimates recommended to be used**. Secondly, estimates for an in-place sensitivity test using a 1,000 ft (305 m) depth cut-off are examined.

### 2. Best technical case in-place gas calculation

The total gas content of a shale is made up of two main components:

**Free gas** – the gas contained in pore spaces; this volume is very pressure dependent, and pressure is related to depth (assuming no overpressure).

Adsorbed gas – the gas which is adsorbed in the organic matter in the shale. The quantity of gas adsorbed is dependent on the quantity, type and distribution of the organic content within the shale; it is largely pressure independent.

In the USA shale gas plays, the ratio of adsorbed gas to free gas varies from 60:40 to 10:90 (Jarvie 2012a).

<sup>&</sup>lt;sup>1</sup> P10, P50 and P90 correspond to the 10%, 50% or 90% probability of more than that amount being present. In the case of P10, there is a 10% probability that the actual result will be higher, or a 90% chance the result will be lower.

#### **Equations** 2.1

 $GIIP_a = A * h * \rho * G$ 

G:

Free gas at standard conditions is calculated using the equation:

 $GIIP_f = A * h * \phi * Bg$ Where A = areah = thickness  $\phi$  = gas-filled porosity B<sub>g</sub> = gas expansion factor (depth dependent)

Adsorbed gas is calculated using the equation:

Where A = area h = thickness  $\rho = \text{rock density}$ G = adsorbed gas content of shale (volume of gas/weight of shale) Where experimental analysis of core samples is available, the Langmuir equation is used to calculate

G = <u>G<sub>l</sub> \* P</u>  $P_1 + P$ 

Where  $G_1$  = Langmuir volume [volume of adsorbed gas at infinite pressure]

 $P_1$  = Langmuir pressure [pressure where one-half of the gas at infinite pressure has been desorbed]

P = Reservoir pressure

Total gas in place (GIIP) (at standard conditions) = Free gas (GIIP<sub>1</sub>) + Adsorbed gas (GIIP<sub>2</sub>)

#### Values used 2.2

#### 2.2.1 Free gas

The controlling factors for free gas are area, thickness, gas-filled porosity and depth (and overpressure, if present). Those factors that are estimated in this study are shown in bold; those that rely on analogues are shown in italics.

Rather than inputting parameters for area and thickness separately, figures for the net organic-rich, mature shale volumes have been used. These are the volumes of organic-rich shale (TOC>2%) which are considered mature for gas generation ( $R_0>1.1$ ). Further explanation of how these volumes were derived can be found in Section 4.1 of the main report.

Specific information on the gas-filled porosities of Midland Valley of Scotland shales is limited. O'Donnell (2013) used a porosity of 5-6% and a gas saturation of 85% (gas-filled porosity = 4.3 -5.1%) for the West Lothian Oil-Shale unit and Reach used a porosity of 5% (based on an average total porosity of 7.9%) in their resource calculations (pers. comm.). Data from shallow West Lothian Oil-Shale cores had a gas-filled porosity of 1.4 - 5.5 %. (Reach pers. comm.). Significant kerogen porosity of 12%, as measured on a whole rock basis, could develop with maturity of the kerogen (Reach pers. comm.). This kerogen porosity system will have no water saturation and the magnitude of this system will be a factor of maturity, transformation ratio of the kerogen and original TOC (Jarvie

2012c). Reported gas-filled porosities for US gas shales are in the range 1-5% (Curtis 2002) and 2.9-6% (Jarvie 2012a). Lewis *et al.* (2004) quotes a figure of 4-6% porosity for gas shales. For an undeveloped play in the Netherlands, TNO (2009) used the Curtis (2002) figures of 1-5% gas-filled porosity. These conservative figures are used in this analysis (as in Andrews 2013): a log-normal distribution with a mean of 3% porosity and a two standard-deviation variation with cut-offs at 0.5% and 10%.

The gas expansion factor  $(B_g)$  converts the volume of free gas under reservoir conditions into a volume under atmospheric conditions using the formula:

 $B_g = depth(m)/10.7$ 

It is not known whether the Scottish shales are overpressured, and hydrostatic pressure has been assumed. Any overpressure would increase the quantity of free gas stored in the pore spaces. Shale gas accumulations in the USA are commonly overpressured.

#### 2.2.2Adsorbed gas

The controlling factors are **area**, **thickness**, **shale density** and *adsorbed gas content of shale*. Those factors that are estimated in this study are shown in bold; those that rely on analogues are shown in italics.

Langmuir volumes can be obtained experimentally from core samples, but none have been published for shales in Scotland. Published values of adsorbed gas contents of shales in the USA are as follows:

Source	Basin/area	Gas-filled	Total gas	Adsorbed	Adsorbed	Adsorbed
		porosity	content	gas (%)	gas content	gas content
		(%)	(scf/ton)		(scf/ton)	(m³/ton)
Curtis (2002)	Antrim	4	40 - 100	70	28 - 70	0.8 - 2.0
Curtis (2002)	Ohio	2	60 - 100	50	30 - 50	0.8 - 1.4
Curtis (2002)	New Albany	5	40 - 80	40 - 60	16 - 32	0.5 - 0.9
Curtis (2002)	Barnett	2.5	300 - 350	20	60 - 70	1.7 - 2.0
Curtis (2002)	Lewis	1 - 3.5	15 - 45	60 - 85	9 - 27	0.3 - 0.8
Jarvie (2012a)	Marcellus	4	60 - 150	45	27 - 67.5	0.8 - 1.9
Jarvie (2012a)	Haynesville	6	100 - 330	25	25 - 82.5	0.7 - 2.3
Jarvie (2012a)	Bossier	4	50 - 150	55	27.5 - 82.5	0.8 - 2.3
Jarvie (2012a)	Barnett	5	300 - 350	55	165 - 192.5	4.7 - 5.5
Jarvie (2012a)	Fayetteville	4.5	60 - 220	50 - 70	30 - 110	0.8 - 3.1
Jarvie (2012a)	Muskwa	4	90 - 110	20	18 - 22	0.5 - 0.6
Jarvie (2012a)	Woodford	3	200 - 300	60	120 - 180	3.4 - 5.1
Jarvie (2012a)	Eagle Ford	4.5	200 - 220	25	50 - 55	1.4 - 1.6
Jarvie (2012a)	Utica	2.9	70	60	42	1.2
Jarvie (2012a)	Montney	3.5	300	10	30	0.8

Table 1. Summary of parameters for various shales in the USA that are relevant to gas resource calculations in this study (from Curtis 2002, Jarvie 2012a).

For the modelling undertaken in this report (as in Andrews 2013), a fairly conservative range of adsorbed gas contents of 0.5 to 2.0  $\text{m}^3$ /ton (18-71 scf/ton) has been taken.

Published rock densities for Midland Valley of Scotland Carboniferous strata are in the range 2.34-2.72 g/cm<sup>3</sup> (McLean 1961; Qureshi 1970). This study follows Andrews (2013) and uses 2.55 – 2.6 – 2.65 g/cm<sup>3</sup> as a range of values for Carboniferous shale. The use of this range is supported by downhole geophysical well logs in the study area (e.g. the Kilconquhar Mains well in Vincent *et al.* 2010).

### 2.3 Monte Carlo input parameters

	Net mature shale volume (x10 <sup>9</sup> m <sup>3</sup> )			Med	ian dept	h (m)	Gas-filled porosity (%)		
	Low	Central	High	min	ml	max	cut-off	mean	cut-off
	(P95)	(P50)	(P10)						
Limestone Coal	5.8	16.0	24.7	813	1151	1700	0.5	3	10
Fm									
Lower	20.7	30.0	39.4	809	1016	1970	0.5	3	10
Limestone Fm									
West Lothian	65.1	123.0	168.0	804	1050	4505	0.5	3	10
Oil-shale unit									
Gullane unit	32.0	106.0	168.7	809	1570	5469	0.5	3	10

#### For free gas-in-place (GIIP<sub>f</sub>)

#### For adsorbed gas-in-place (GIIP<sub>a</sub>)

	-							
	Net matu	re shale volu	ume (x10 <sup>9</sup>	Der	sity (g/o	cm³)	Adsorbed gas content (m <sup>3</sup> /t)	
		m³)						
	Low	Central	High	min	ml	max	min	max
	(P95)	(P50)	(P10)					
Limestone Coal	5.8	16.0	24.7	2.55	2.6	2.65	0.5	2
Fm								
Lower	20.7	30.0	39.4	2.55	2.6	2.65	0.5	2
Limestone Fm								
West Lothian	65.1	123.0	168.0	2.55	2.6	2.65	0.5	2
Oil-shale unit								
Gullane unit	32.0	106.0	168.7	2.55	2.6	2.65	0.5	2

Table 2. Input parameters for the Monte Carlo simulation used to determine the total gas content and total gas in-place in four Carboniferous subdivisions in the Midland Valley of Scotland.

(a) Metric	Total g	as content e (m³/m³)	stimates	Total gas in-place estimates (tcm)			
	Low (P90)	Central (P50)	High (P10)	Low (P90)	Central (P50)	High (P10)	
Limestone Coal Fm	2.9	5.8	10.3	0.04	0.09	0.17	
Lower Limestone Fm	2.9	5.8	10.5	0.10	0.18	0.31	
West Lothian Oil-shale unit	3.4	7.6	15.7	0.46	0.92	1.89	
Gullane unit	3.9	8.7	18.4	0.36	0.91	2.07	
Combined				1.40	2.27	3.81	

### 2.4 Monte Carlo results

	-						
(b) Imperial	Total g	as content e (bcf/mile <sup>2</sup> m	estimates	Total gas in-place estimates (tcf)			
	Low Central High (P90) (P50) (P10)		Low (P90)	Central (P50)	High (P10)		
Limestone Coal Fm	0.26	0.53	0.94	1.4	3.2	6.1	
Lower Limestone Fm	0.26	0.53	0.96	3.7	6.3	10.8	
West Lothian Oil-shale unit	0.31	0.69	1.43	16.2	32.6	66.7	
Gullane unit	0.36	0.80	1.67	12.5	32.0	73.2	
Combined				49.4	80.3	134.6	

Table 3. Results of a Monte Carlo simulation (500,000 iterations) to determine the total gas content and total in-place gas resource in four Carboniferous subdivisions in the Midland Valley of Scotland. The results are given in (a) metric and (b) imperial units. Note that the 'combined' resource figures are the result of a separate Monte Carlo simulation, they are not the sum of the four subdivisions.

In the results Table 3 and in Tables 6, 9, 11 below, the 'combined' resource figures are the result of a separate Monte Carlo simulation; because the resource figures are the P10-P50-P90 outputs of a statistical distribution it is not valid to sum the four subdivisions to give a combined figure.

The 'combined' Monte Carlo simulation gives a narrower range than would a sum of the subdivisions because combining the distributions stochastically reduces the coefficient of variation (the standard deviation divided by the mean). That is reflected by the smaller difference between the P90 and P10 figures in the combined run. In a normal distribution, the sum of the P50 subdivisions would be expected to be the same as the 'combined' P50 simulation, however, the distributions have been skewed towards P90 (low end; Figure 1) to account for uncertainties within the input data, such that this is not the case.



Figure 1 Probabilistic distributions representing the results of a Monte Carlo analysis for the in-place resource estimation of shale gas in four Carboniferous shale units of the Midland Valley of Scotland (separate and lastly combined).

Variable	Uncertainty
Gross rock volume/3D geological model	The 2D seismic data interpreted in the study area is of variable quality, and is generally poor to moderate. The mapping of the Gullane unit is more uncertain than the overlying units. The distribution was skewed to the lower end to accommodate uncertainties in the input parameters.
Definition of prospective shale	In the heterogeneous strata of the Midland Valley of Scotland, the definition of net prospective shale used in this report has two end-members. As a maximum, all organic-rich shales are included, independent of bed thickness. At the lower end, only shales occurring in units at least 50 ft thick are included. This methodology contrasts with the more uniform fine-grained successions in the Bowland-Hodder and Weald studies, for which bed thickness is not an issue.
Definition of gas maturity	The use of $R_o > 1.1\%$ as the top of the gas window is possibly optimistic. It could be $R_o > 1.4\%$ which would reduce the estimated gas volume.
Shallow depth cut-off	The use of depth cut-offs is discussed in the main report. If this were deeper, this would reduce the estimated gas volume, and <i>vice versa</i> .
Gas-filled porosity of the shale	The use of a mean of 3% is a conservative estimate. It could be greater, which would increase the estimated gas volume. The large range of values used has a significant effect on the calculated in-place gas figure (see Figure 2).
Reservoir pressure	The assumption that the shales are at hydrostatic pressure is conservative. Any amount of overpressure would increase the estimated gas volume.
Adsorbed gas content	The use of 0.5-2.0 m <sup>3</sup> /ton is lower than some US analogues. Any increase in this range of values would increase the estimated gas volume.
Bulk density	The average density of 2.6 g/cm <sup>3</sup> is a robust estimate. If the density is higher this will increase the estimated gas volume (and vice versa).

### 2.5 Key variables and their effect on the estimated gas volume

this will increase the estimated gas volume (and vice versa).Table 4. Key variables and their effect on the estimated gas volume



Figure 2. Tornado diagrams representing the result of a Monte Carlo analysis for the in-place resource estimation of shale gas in the four Carboniferous shale units of the Midland Valley of Scotland.

### **3** Best technical case in-place oil calculation

As in the Weald Basin of southern England (Andrews 2014), the paucity of geochemical data in the Midland Valley of Scotland precludes a full understanding of free oil contents that should be necessary to estimate in-place resources. However, in contrast to the Weald Basin, there is less reason to suggest that most/all of the measured S1 is associated with kerogen (i.e. there is a poor relationship between TOC and S1, see cross-plot main report Figure 53). Therefore, the entire S1 peak is considered to be free oil. This is then corrected for evaporative loss (see Michael *et al.* 2013) and used as the free oil density.

### **3.1 Equations**

This report follows Andrews (2014) and converts the S1 data from Rock-Eval analyses to an estimation of free oil yield to determine oil in-place, using Michael *et al.*'s (2013) equation:

Oil in-place (bbls/acre-ft) = corrected S1 (mgHC/gRock) x rock density (g/cm<sup>3</sup>)  $\div$  oil density (g/cm<sup>3</sup>) x unit conversion factor

The unit conversion factor to convert from  $cm^3/m^3$  to bbl/acre-ft = 7.758

### 3.2 Values used

The values for the net 'accessible/viable', oil-mature, organic-rich shale volume are calculated using the same methodology as for gas-mature shales, but using a depth envelope approximating to between  $R_0 = 0.6$  and 1.1.

Present day S1 values are taken from Rock-Eval analyses in organic-rich shales (see Table 6 of the main report). The S1 values used are restricted to those samples with a TOC of 2-30% (i.e. organic-rich, but excluding coals) and  $R_o <= 1.1\%$  (i.e. shallower than the gas window). This 'free oil density' is the amount of the original S1 that is considered to represent extractable oil. The minimum case is that a minimal amount of the S1 oil is free oil (with the remainder bound within the kerogen). The most-likely and maximum cases assume that all the S1 will be 'free oil', but in the analyses has been reduced by evaporative loss.

The evaporative loss of S1 from the samples over time may have been considerable, especially if more volatile oils are concerned. For a selection of source rock types and basins, Michael *et al*. (2013) propose the equation:

% C<sub>15</sub> minus lost = (oil API – 20.799)/0.412

For API = 35°, loss is 34.5%; API = 40°, loss is 46.4%; API = 45°, loss is 58.7%. The corresponding correction factors are 1.53, 1.87 and 2.42 respectively.

Other authors consider that evaporative loss can be a more significant issue, with correction factors up to 4.0 or even 5.0 suggested by Jarvie *et al.* (2012b). There is no evidence of high API oils in the Midland Valley of Scotland area which are most likely to require such large corrections.

The shale densities used are the same as for the gas calculation (section 2.3).

Oil density or specific gravity (g/cm<sup>3</sup>) = 141.5/(131.5 + oil API) (American Petroleum Institute definition). The range used in this report is for 35°, 40° and 45° API oil. There is little available information on the gravity of oils in the conventional discoveries of the Midland Valley of Scotland. A sample of waxy oil from Milton of Balgonie 1 had a specific gravity of 36.73° API at 60°F (company well report).

	Accessi	ble/viable\$	volume	Free	oil cor	ntent	Co	Correction for		Shale density (g/cm <sup>3</sup> )		(/cm³)	Oil density (g/cm <sup>3</sup> )		
	of net organic-rich mature		(mg	(mgHC/gRock)		eva	porative	loss							
	shale (x10 <sup>9</sup> m <sup>3</sup> )														
	Low	Central	High	min	ml	max	min	ml	max	min	ml	max	min	ml	max
	(P95)	(P50)	(P10)												
Limestone Coal	7.1	15.0	24.9	0.1	1.40	3.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
Fm															
Lower Limestone	12.5	19.0	25.7	0.1	0.57	2.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
Fm															
West Lothian Oil-	21.8	48.0	77.3	0.1	1.52	6.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
shale unit															
Gullane unit	6.7	15.0	25.6	0.1	0.29	1.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85

### 3.3 Monte Carlo input parameters

Table 5. Input parameters for the Monte Carlo simulation used to determine the total oil in-place in four Carboniferous subdivisions in the Midland Valley of Scotland. \$ = volume of shale below various depth cut-offs.

### **3.4 Monte Carlo results**

(i) Metric	Total oil in-pla	ace estimates (m	nillion tonnes)
	Low (P90)	Central	High (P10)
		(P50)	
Limestone Coal Fm	42	106	221
Lower Limestone Fm	35	78	153
West Lothian Oil-shale	192	542	1,241
unit			
Gullane unit	13	32	70
Combined	421	793	1,497

(ii) Imperial	Total oil in-	place estimates	(billion bbl)
	Low (P90)	Central	High (P10)
		(P50)	
Limestone Coal Fm	0.32	0.79	1.65
Lower Limestone Fm	0.26	0.59	1.15
West Lothian Oil-shale	1.44	4.07	9.26
unit			
Gullane unit	0.10	0.24	0.53
Combined	3.2	6.0	11.2

Table 6. Results of a Monte Carlo simulation (50,000 iterations) to determine the total in-place oil resource in four Carboniferous units in the Midland Valley of Scotland. The results are given in (i) metric and (ii) imperial units. Note that the 'combined' resource figures are the result of a separate Monte Carlo simulation, they are not the sum of the four subdivisions.



Figure 3. Probabilistic distributions representing the results of a Monte Carlo analysis for the in-place resource estimation of shale oil in four Carboniferous shale units of the Midland Valley of Scotland (separate and lastly combined).

### 3.5 Key variables and their effect on the estimated oil volume

Variable	Uncertainty
Gross rock volume/3D geological model	As for gas.
Shallow depth cut-off	As for gas.
Definition of prospective shale	As for gas.
Free oil density	Oil yields are controlled by kerogen type, percentage of free or extractable oil and the amount of evaporative loss affecting S1 peaks. If the samples have undergone higher evaporative loss than predicted, then the estimates could be low.
Definition of oil maturity	The use of $R_o = 0.6\%$ as the top of the oil window is standard practice. It could be 0.7% which would reduce the estimated oil volume, or 0.5% which would increase it. The base of the oil window is discussed above in relation to the top of the gas window.
Bulk density	As for gas.





*Figure 4. Tornado diagram representing the result of a Monte Carlo analysis for the in-place resource estimation of shale oil in the four Carboniferous shale units of the Midland Valley of Scotland.* 

### 4. Sensitivity test using 1,000 ft depth cut-off

A large swathe of central and central-eastern Scotland is estimated to be underlain by organic rich shale strata mature for shale-oil and shale-gas at relatively shallow depths, so a sensitivity using a 1,000 ft depth-cut off was also examined. The best technical case extent and volume of shale likely to be potentially exploitable once historic deep mining and standard depth criteria are taken into account is smaller (see above).

Historic deep mining is one reason why the 1,000 ft cut-off is used only as a sensitivity test. Other reasons include gas pressure and groundwater considerations, thus it is important to note that:

- The 1,000 ft sensitivity test resource figures include volumes which have been effectively sterilised by historic deep mining
- The 1,000 ft cut off is significantly shallower than the 3,300 ft used by USEIA (2013) for a successful shale play.
- The shallowest part of the volume is within the 400 m zone of 'groundwater bodies'

Apart from the net mature shale volume and median depth (gas calculation), the input parameters and methodology for the maximum case sensitivity test are the same as described above.

### 4.1 Shale gas Monte Carlo input parameters

1,000 ft depth	Net matu	re shale volu m <sup>3</sup> )	ume (x10 <sup>9</sup>	Med	ian dept	h (m)	Gas-filled porosity (%)		
	Low (P95)	Central (P50)	High (P10)	min	ml	max	cut-off	mean	cut-off
Limestone Coal Fm	9.4	21.8	36.5	305	643	1643	0.5	3	10
Lower Limestone Fm	28.6	40.2	55.9	305	932	1906	0.5	3	10
West Lothian Oil-shale unit	83.4	143.6	218.8	480	1077	4503	0.5	3	10
Gullane unit	52.8	126.4	213.3	558	1537	5466	0.5	3	10

#### For free gas-in-place (GIIP<sub>f</sub>)

#### For adsorbed gas-in-place (GIIP<sub>a</sub>)

1,000 ft depth	Net matu	re shale volu	ume (x10 <sup>9</sup>	Den	isity (g/o	cm³)	Adsorbed gas content (m <sup>3</sup> /t)	
cut-off								
	Low	Central	High	min	ml	max	min	max
	(P95)	(P50)	(P10)					
Limestone Coal	9.4	21.8	36.5	2.55	2.6	2.65	0.5	2
Fm								
Lower	28.6	40.2	55.9	2.55	2.6	2.65	0.5	2
Limestone Fm								
West Lothian	83.4	143.6	218.8	2.55	2.6	2.65	0.5	2
Oil-shale unit								
Gullane unit	52.8	126.4	213.3	2.55	2.6	2.65	0.5	2

Table 8 Input parameters for the Monte Carlo simulation used to determine the total gas content and total gas in-place in four Carboniferous subdivisions in the Midland Valley of Scotland using a 1000 ft depth-cut off.

(a) Metric	Total g	as content e (m³/m³)	stimates	Total gas in-place estimates (tcm)					
1,000 ft depth cut-off	Low (P90)	Central (P50)	High (P10)	Low (P90)	Central (P50)	High (P10)			
Limestone Coal Fm	2.9	2.9 5.8		0.05 0.10		0.21			
Lower Limestone Fm	2.9	5.8	10.5	0.12	0.22	0.38			
West Lothian Oil-shale unit	3.4	7.6	15.7	0.53	1.07	2.30			
Gullane unit	3.9	8.7	18.4	0.45	1.07	2.52			
Combined				1.66	2.70	4.63			

### 4.2 Shale gas Monte Carlo results

(b) Imperial	Total g	as content e	estimates	Total gas in-place estimates (tcf)					
		(bcf/mile <sup>2</sup> m	ı)						
1,000 ft depth cut-off	Low	Central	High	Low (P90)	Central (P50)	High (P10)			
	(P90)	(P50)	(P10)						
Limestone Coal Fm	0.26	0.53	0.94	1.7	3.7	7.3			
Lower Limestone Fm	0.26	0.53	0.96	4.4	7.6	13.5			
West Lothian Oil-shale	0.31	0.69	1.43	18.6	37.9	81.2			
unit									
Gullane unit 0.36 0.80 1				15.9 37.9 89.0					
Combined				58.7	95.4	163.5			

Table 9 Results of a Monte Carlo simulation (500,000 iterations) to determine the total gas content and total in-place gas resource in four Carboniferous subdivisions in the Midland Valley of Scotland using a 1000 ft depth-cut off. The results are given in (a) metric and (b) imperial units. Note that the 'combined' resource figures are the result of a separate Monte Carlo simulation, they are not the sum of the four subdivisions.

### 4.3 Shale oil Monte Carlo input parameters

1,000 ft depth cut-off	Accessible/viable\$ volume of net organic-rich mature shale (x10 <sup>9</sup> m <sup>3</sup> )				Accessible/viable\$ volumeFree oil contentCorrection forof net organic-rich mature(mgHC/gRock)evaporative lossshale (x10 <sup>9</sup> m³)			Shale density (g/cm <sup>3</sup> )			Oil density (g/cm <sup>3</sup> )				
	Low (P95)	Central (P50)	High (P10)	min	ml	max	min	ml	max	min	ml	max	min	ml	max
Limestone Coal Fm	27.4	57.9	94.4	0.1	1.40	3.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
Lower Limestone Fm	38.9	56.0	79.0	0.1	0.57	2.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
West Lothian Oil- shale unit	44.4	96.1	157.8	0.1	1.52	6.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85
Gullane unit	17.0	42.4	72.2	0.1	0.29	1.0	1.53	1.87	2.42	2.55	2.6	2.65	0.8	0.825	0.85

Table 10. Input parameters for the Monte Carlo simulation used to determine the total oil in-place in four Carboniferous subdivisions in the Midland Valley of Scotland using a 1000 ft depth-cut off. \$ = volume of shale below various depth cut-offs.

(i) Metric	Total oil in-place estimates (million tonnes)								
1,000 ft depth cut-off	Low (P90)	Central	High (P10)						
		(P50)							
Limestone Coal Fm	163	407	839						
Lower Limestone Fm	104	235	462						
West Lothian Oil-shale	387	2,516							
unit									
Gullane unit	35	89	198						
Combined	1,116	1,948	3,418						

### 4.4 Shale oil Monte Carlo results

(ii) Imperial	Total oil in-place estimates (billion bbl)							
1,000 ft depth cut-off	Low (P90)	Central	High (P10)					
		(P50)						
Limestone Coal Fm	1.22	3.05	6.29					
Lower Limestone Fm	0.78	1.76	3.47					
West Lothian Oil-shale	2.90	8.15	18.9					
unit								
Gullane unit	0.26	0.67	1.48					
Combined	8.4	14.6	25.6					

Table 11. Results of a Monte Carlo simulation (50,000 iterations) to determine the total in-place oil resource in four Carboniferous units in the Midland Valley of Scotland using a 1000 ft depth-cut off. The results are given in (i) metric and (ii) imperial units. Note that the 'combined' resource figures are the result of a separate Monte Carlo simulation, they are not the sum of the four subdivisions.

### 4.5 Areal extent

The extent maps for the 1,000 ft depth cut-off are complex (Figures 5,6), with holes where mature volumes are truncated upwards by the 1,000 ft depth cut-off and/or where strata are cut by the oil to gas maturity depth surface ( $R_o$ =1.1%). Summary maps are presented in the main report (Figures 72, 73).



Figure 5 Summary of areas prospective for shale gas in the Limestone Coal and Lower Limestone formations, West Lothian Oil-Shale and Gullane units using the sensitivity case of 1,000 ft depth cutoff.



*Figure 6 Summary of areas prospective for shale oil in the Limestone Coal and Lower Limestone formations, West Lothian Oil-Shale and Gullane units using the sensitivity case of 1,000 ft cut-off.* 

The larger areal extents using the 1,000 ft depth cut-off reflect the shallow depth of mature shale oil- and shale gas-in-place in the subsurface (Figures 5, 6). The extents for shale-oil in particular are much larger than for the mining-related depth cut off (main report section 4) because strata mature for shale oil are commonly buried at depths between the 1,000 ft depth cut-off and the mining-related depth cut-off the shallower 1,000 ft cut off can be seen in the much larger areal extents of the Limestone Coal Formation, Lower Limestone Formations and West-Lothian Oil-Shale unit in the southern and western parts of the Central Coalfield.

### 4.6 Discussion

For shale-oil, comparison of the best technical case and 1,000 ft sensitivity test resource estimates shows that the deeper depth-cut off of the former, which significantly reduces net oil-mature shale volumes, has a large effect (Figure 7). The best technical case P50 value is less than the 1,000 ft sensitivity test P90 value. This is because over large parts of the area, strata mature for shale oil are buried at depths between the 1,000 ft depth cut-off and the mining-related depth cut-off at 2,640+ ft. The Limestone Coal and Lower Limestone formations make up a large proportion of the net mature strata between the cut-off depths and thus their percentage increase in contribution to the overall 1,000 ft sensitivity test shale oil resource estimate are proportionately greater than the West Lothian Oil-Shale and Gullane units (Table 1). However, it is important to note that significant parts of the volume between the depth cut-offs is effectively sterilised by historic mine workings, many in the Limestone Coal Formation (see main report section 4). Future work could examine mining, geomechanical, geochemical and hydrogeological data at the local scale, to assess the potentially large shale-oil resource between the 1,000 ft (305 m) and 2,640+ ft (805+ m) cut-off depths in greater detail.





For shale-gas, comparison of the best technical case and 1,000 ft depth cut-off sensitivity test resource estimates shows that the deeper depth-cut off of the former, which reduced net gasmature shale volumes, has a relatively small effect (Figure 8). This is because over a lot of the area, strata mature for shale gas are buried beneath both depth cut-offs.



*Figure 8 Comparison of combined shale gas resource estimates for the 1,000 ft depth cut-off sensitivity test and the best technical case with a deeper mining-related cut-off.* 

# **5** Conclusions

The figures given are for the best technical case of potentially exploitable shale-oil and shale-gas using a mining-related depth cut-off (see main report, section 4)

This study estimates that the **total in-place gas resource** for the Carboniferous shales across the Midland Valley of Scotland is **49.4 – 80.3 – 134.6 tcf** (1.40 – 2.27 – 3.81 tcm) (P90 – P50 – P10).

It is also estimated that the **total in-place oil resource** for the Carboniferous shales across the Midland Valley of Scotland is **3.2** – **6.0** – **11.2 billion bbl** (421 – 793 – 1,497 million tonnes) (P90 – P50 – P10).

In order of significance, the West Lothian Oil-Shale unit contributes the largest in-place resource in this model, followed by the Gullane unit.

It should be emphasised that whilst a mining-related depth-cut off has been used to narrow the potentially exploitable resource from that which is present in the subsurface, these figures are inplace resource estimates. The amount of oil and/or gas that could be recovered depends on factors outwith the scope of this report, and could very likely be a small percentage.

### **6 References**

See main report.

# Appendix B. Additional detail on Midland Valley of Scotland stratigraphy, magmatism and tectonism

A.A. Monaghan & M.A.E. Browne

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# **1** Areas excluded from shale prospectivity study

This section provides the background detail on why some areas of the Midland Valley of Scotland were excluded from the resource estimation (see main report Figure 2).

### 1.1 Western Midland Valley of Scotland – Ayrshire and Douglas Coalfields

There are significant differences in the Ayrshire and Douglas Carboniferous stratigraphical sequence to that of the central and eastern Midland Valley of Scotland. The Clyde Plateau Volcanic Formation, unconformities and/or a very thin succession characterise much of the Strathclyde Group where it is known at outcrop or in boreholes. There are no deep geophysical well data and only 34 boreholes in the BGS database greater than 1640 ft/500 m drilled depth.

Strata of the Coal Measures and Clackmannan Group are most deeply buried under the Permian Mauchline Basin, where over 2,130 ft (650 m) of heterogeneous Coal Measures strata are recorded in three BGS borehole records. Former deep coal mining of these strata is extensive.

Clackmannan Group strata are of very variable thickness, being completely missing to the south of Ayr (Smith *et al.* 2013) and thicker in north Ayrshire (Monro 1999). The Kilbirnie Mudstone Member reaches around 150 ft (45 m) thick at the base of the Limestone Coal Formation in north Ayrshire (Monro 1999) but is not likely to be buried more deeply than 1,640 ft (500 m) (Monaghan 2013).

The Clyde Plateau Volcanic Formation and the overlying largely volcaniclastic Kirkwood Formation dominate the Strathclyde Group (Monro 1999). The Lawmuir Formation is often absent in north Ayrshire (Monro 1999). In south Ayrshire the Lawmuir Formation reaches up to 330 ft (100 m) and is sandstone dominated (Smith *et al.* 2013). There is no mudstone-rich equivalent of the West Lothian Oil-Shale Formation.

The Invercive Group commonly contains unconformities. In south Ayrshire typical facies of the Ballagan Formation (mudstone, dolostone, siltstone, thin sandstone) reach up to 1,310 ft (400 m) to the south of Ayr (Smith *et al.* 2013). However these strata are proven only to the shallow subsurface and there is no information on their extent at depth, or on their organic content.

In the Douglas Coalfield, any development of the Inverclyde and Strathclyde groups is limited in occurrence, thin and locally absent. The Lawmuir Formation is present with at least one marine limestone developed. The succession is of sandstone with some mudstone, but these are pale coloured. The full Clackmannan Group succession is developed and each formation is relatively thin, but there are abnormally rich in thick coal seams. Mudstone is well developed in the lower half of the Limestone Coal Formation and throughout the Upper Limestone Formation. However, these rocks are not buried at depths of interest to this study.

In summary, the Ayrshire and Douglas Coalfield areas of the western Midland Valley of Scotland are not considered as prospective for shale due to the lack of organic-rich mudstone-dominated strata at suitable depth, plus the lack of deep well data and associated information.

### **1.2 Devonian strata**

Sandstone, conglomerate and volcanic rock are the dominant lithologies of Early and Late Devonian strata on the northern and southern sides of the Midland Valley of Scotland (Browne *et al.* 2004). The Dundee Flagstone Formation contains minor siltstones and mudstones, some of which have TOC up to 0.93% (Robinson *et al.* 1989). However, there is no data to constrain their westward extent at depth (Robinson *et al.* 1989) and as the TOC is less than 2% these strata were not considered further.

### 1.3 Inliers of the southern Midland Valley of Scotland

Silurian and Ordovician strata crop out in inliers at the margins of the Midland Valley of Scotland, with some formations containing mudstones (Cameron & Stevenson 1985). There are no data to constrain the thickness and geometry of these mudstones in the subsurface and they are likely to be heavily faulted; thus these strata were not considered further.

# 2 Stratigraphic constraints

Palaeogeographic maps (main report) form an important basis for estimating the distribution of shale and the extent of volcanic strata. The timing of events in the palaeogeographic reconstructions (main report Figures 27, 32, 33, 38) was taken from an integrated chrono- and biostratigraphical chart (Figure 1).

In the Midland Valley of Scotland, biostratigraphical correlation can generally be identified to stage level, even in the dominantly non-marine Lower Carboniferous rocks where palynology provides the main biostratigraphical control. Marine fossils are stratigraphically important from the late Asbian with the appearance of a number of marine bands with rich faunas known collectively as the Macgregor Marine Bands. Non-marine bivalve macrofossils, *Paracarbonicola* sp, *Naiadites obesus* and *Curvirimula scotica*, mark broad zones within the Asbian and Brigantian strata, with *Curvirimula* replacing *Naiadites* at about the level of the Burdiehouse Limestone. Igneous rocks have been dated by U-Pb and <sup>40</sup>Ar/<sup>39</sup>Ar radiometric methods to form a numerical time framework (e.g. Monaghan et al. in press, Figure 1). Figure 1 also shows how the Western European chronostratigraphy fits with the international Mississippian Epoch.



Figure 1 Magmatic time chart, plotted on a linear GTS2012 timescale (Davydov et al. 2012) with UK stage names from British Geological Survey (2013b), modified after Monaghan et al. (in press; Scottish Journal of Geology). Wells constraining volcanic strata are shown as vertical blue lines, though because the chart summarises igneous activity at many geographical locations the full stratigraphy of the wells is not represented. Modelled depth horizons here shown as red lines.

Stratigraphic nomenclature across the Midland Valley of Scotland varies from area to area. As there is limited published information on correlations within the Strathclyde Group, a summary of local names is illustrated here (Figure 2). This was used to assist in stratigraphical well interpretations (Appendix C).



Figure 2 Correlation of marine bands and limestones in the Strathclyde Group

# **3 Tectonic and magmatic basin evolution**

This section is included to give an insight into the current day arrangement of basins, faults and igneous rocks in the Midland Valley of Scotland.

# 3.1 Late Devonian to Early Carboniferous basin formation in the Variscan foreland

The extensional to strike-slip Midland Valley of Scotland forms part of a system of Late Devonian to Carboniferous sedimentary basins that developed across northern Britain in the foreland of the Variscan Orogen (Ziegler 1990). Several different regional tectonic models have been proposed: back-arc extension in relation to northwards subduction of the Rheic Ocean lithosphere (Leeder 1982); dextral megashear during accretion of Gondwana and Laurentia that stretched from North America to Russia (Arthaud & Matte 1977, Dewey 1982); or dextral escape tectonics of a continental block during the Early Carboniferous with sinistral strike-slip movement over the area of the Midland Valley of Scotland terrane, followed by Late Carboniferous reversal of the escaping continental block resulting in dextral strike-slip across northern Britain (Coward 1993).

In the Midland Valley of Scotland, Late Devonian to Early Carboniferous (Tournaisian) NE-trending extensional depocentres (Browne & Monro 1989) were followed in one model by Visean N-S extensional faults in response to a sinistral strike-slip tectonic regime (Rippon *et al.* 1996, Ritchie *et al.* 2003), compatible with the regional model of Coward (1993). In the eastern Midland Valley of Scotland, an alternative model proposes NNE-trending growth synclines and anticlines from the mid to late Visean, related to dextral strike-slip tectonics (Underhill *et al.* 2008, Monaghan *et al.* 2012), compatible with regional wrench models such as that of Dewey (1982). Outcrop-based studies from the western Midland Valley of Scotland synthesise movements on NE, N and NW trending faults, plus N-S and E-W folds to sinistral strike-slip and extension in the Early Carboniferous, followed by

dextral movement and compression during the Late Carboniferous, compatible with the Coward (1993) plate reconstruction (Caldwell & Young 2013).

The eruption of the Clyde Plateau Volcanic Formation was controlled by NE- to ENE- and conjugate NW-trending structures (Hall *et al.* 1998, Monro 1999). A Chadian–early Asbian unconformity developed across much of the Midland Valley of Scotland (Browne & Woodhall 1999, Read *et al.* 2002, Stephenson *et al.* 2004, Waters *et al.* 2011b). However, due to burial beneath younger strata and overprinting by succeeding tectonism, the Visean fault pattern is poorly constrained.

### 3.2 Mid to Late Carboniferous basin formation to inversion

In mid- to late Carboniferous time, dextral strike-slip tectonics in the Midland Valley of Scotland are commonly interpreted (Read 1988, Rippon *et al.* 1996, Ritchie *et al.* 2003, Underhill *et al.* 2008), followed by more compressional structures towards the climax of the Variscan Orogeny (Corfield *et al.* 1996). Leeder (1982) related this to Rheic Ocean closure and final Variscan collision, whereas Coward (1993) proposed that closure of the Ural Ocean caused reversal of the previously escaping continental block.

During Namurian to Westphalian C time, NNE-trending growth synclines and anticlines were active in the eastern and central Midland Valley of Scotland (Read 1988, Ritchie *et al.* 2003) with halfgraben and a horst block bounded by Caledonian E- to NE-trending structures in the western Midland Valley of Scotland (Mykura *et al.* 1967). Significant stratal growth is observed across some east-west faults (e.g. East Ochil Fault, Browne & Woodhall 1999, Monaghan *et al.* 2012).

Tightening of the NNE-trending folds and creation of other N- and NW-trending folds occurred during latest Carboniferous time, resulting in a Westphalian D to Stephanian unconformity (Mykura *et al.* 1967, Rippon *et al.* 1996).

### 3.3 Latest Carboniferous to Permian tholeiitic magmatism and postorogenic extension

Stephanian to Early Permian post-orogenic extension occurred in response to the gravitational collapse of the Variscan Orogen and far-field dextral extensional stress between the Gondwana and Laurentian plates (Ziegler 1990, Timmerman 2004). A widespread phase of latest Carboniferous to Early Permian intrusive tholeiitic magmatism is recognised in north-eastern England, Scotland and across the northern North Sea to the Oslo Graben (Smythe *et al.* 1995, Ernst & Buchan 1997, Neumann *et al.* 2004). From northern Britain to Scandinavia, the approximately east–west orientated structures associated with the tholeiitic magmatic phase are roughly perpendicular to the trend of the regionally extensive NW- to NE- trending rift systems that followed (Coward 1995).

During the Midland Valley of Scotland tholeiitic magmatic phase, ENE-to ESE-trending tholeiitic dykes and extensional faults cut across tightened and inverted Carboniferous basins (Cameron & Stephenson 1985, Rippon *et al.* 1996). Dykes were emplaced along approximately east–west trending fault planes and are also offset by them (Browne & Woodhall 1999, Stephenson *et al.* 2003). Subsequently, latest Carboniferous to Permian alkaline basaltic sills, vents, necks and dykes and one preserved lava succession (Mauchline Volcanic Formation) had an extension-related

petrogenesis (Wallis 1989) and appear to be related to NNE- to NW-trending post-Carboniferous extensional fault systems (Anderson *et al.* 1995, Upton *et al.* 2004).

### 3.4 Post Carboniferous deposition, uplift and erosion

In the Midland Valley of Scotland, the compaction state of the exposed Carboniferous rocks and the presence of late Palaeozoic and Mesozoic successions in parts of Scotland and its offshore waters has led to the hypothesis that the younger successions were deposited and have since been removed by uplift and erosion (e.g. Cameron & Stephenson 1985). For example, Permian and Triassic strata are preserved onshore in the Mauchline Basin, Ayrshire (Mykura *et al.* 1967) and on Arran (BGS 1987). Sequences of Permian and Jurassic rocks up to approximately 5,000 ft (1,500 m) thick are preserved offshore in the outer Firth of Forth/Forth Approaches and in the Firth of Clyde (BGS 1985, Cartwright *et al.* 2001).

Scotland has been subjected to regional uplift since the early Paleocene (Hillis *et al.* 1994) due to magmatic underplating from a mantle plume during the opening of the North Atlantic (White 1988). Thus, sedimentary deposition is likely to have ended at around 60 Ma, coeval with the start of North Atlantic magmatism, uplift and erosion.

Vitrinite relectance data and thermal modelling of well data implies previous burial to depths of approximately 6,000-8,000 ft (2,000-3,000 m) prior to uplift of up to 6,230 ft (1,900 m) (e.g. Vincent *et al.* 2010).

# 4 Stratigraphical summary of Carboniferous units not considered prospective for shale

Descriptions of the non-prospective strata are given here from oldest to youngest, to highlight the logic for their exclusion from the resource estimation, and also to document something of the overburden succession.

### 4.1 Inverclyde Group

The 330-2,100 ft (100-640 m) thick, fluvial Kinnesswood Formation and >980 ft (300 m) thick, fluvial Clyde Sandstone formations are sandstone-dominated with minor pedogenic limestone and red, brown and grey mudstone (Browne *et al.* 1999). The intervening, up to 2,950 ft (900 m) thick, alluvial to marginal marine Ballagan Formation is characterised by grey mudstone and siltstone, nodules and beds of ferroan dolostone and minor sandstone (Browne *et al.* 1999). Given the high percentage of mudstone, likely depth of burial and lateral extent of this formation, it was considered in more detail. However, BGS and existing samples (*e.g.* Turner 1991) give the majority of TOC measurements less than 2% (main report Figure 47), thus the Ballagan Formation does not have sufficient organic carbon content to be included in the current shale resource estimation.

### 4.2 Strathclyde Group

The Strathclyde Group comprises volcanic and sedimentary formations which vary laterally (main report Table 4). Formations containing prospective shales are described in the main report (section 2.9); the remaining formations are summarised here.

The fluvial and lacustrine **Fife Ness Formation** (>755 ft, 230 m thick) is the basal division of the Strathclyde Group in Fife and is dominated by sandstone arranged in upward-fining cycles, with minor argillaceous beds and seatearths (Browne *et al.* 1999).

The Asbian-Brigantian **Aberlady Formation** is up to 460 ft (140 m) thick where it crops out in East Lothian. It consists of a cyclical sequence of sandstone, siltstone and grey mudstone, with subordinate coal, seatrock, limestone, ironstone and marine bands with relatively rich and diverse faunas (Browne *et al.* 1999). The depositional environment was fluvio-deltaic, into lakes and marine embayments. The formation is laterally equivalent to, and has a transitional boundary with, the West Lothian Oil-Shale Formation to the west, being distinguished from it chiefly by the rarity of oil-shales. The Aberlady Formation is identified in the Spilmersford borehole where only around 11% of the succession consists of shale, in beds less than 16 ft (5m) thick.

In the western and central part of the study area, the Asbian-Brigantian Lawmuir Formation is up to 1,083 ft (330 m) thick. It comprises a cyclic sequence of mudstone, siltstone and sandstone, with seatearths, coals and marine limestones (Hall *et al.* 1998). Marine bands are present in the upper part, and conglomerates occur in the lowest parts. The heterogeneous succession was predominantly deposited as fluvial sandstones with overbank mudstones, though there are at least two marine bands and a single 3 ft (1 m) thick oil-shale (Paterson *et al.* 1998, Forsyth *et al.* 1996). With the exception of the approximately 98 ft (30 m) thick 'Dykebar Marls' (poorly-bedded calcareous mudstone) in the Paisley-Hurlet area (Hall *et al.* 1998), mudstone units are thin. Four samples analysed from the Lawmuir Formation show a range of TOC contents from 0.56-2.09 %.

The Lawmuir Formation crops out around the Clyde Plateau Volcanic Formation high and occurs in boreholes to the north and south of Glasgow. Basinward, the formation passes laterally to the West Lothian Oil-Shale Formation, though the boundary is poorly defined (Figure 32, main report).

Up to 118 ft (36 m) of **Kirkwood Formation** overlies the Clyde Plateau Volcanic Formation on the western side of the Central Coalfield; it consists predominantly of volcaniclastic sedimentary rocks.

### 4.3 Clackmannan Group

Upper parts of the Clackmannan Group contain some thick mudstones. However they are generally more shallowly buried than 3,280 ft (1,000 m) onshore and are not currently considered as a prospective shale resource.

The up to 1,970 ft (600 m) thick, Namurian age **Upper Limestone Formation** is characterised by repeated upward-coarsening cycles comprising marine limestone overlain by grey to black mudstones and calcareous mudstones, siltstones and paler sandstones capped by seatrocks and coal (Browne *et al.* 1999). In the upper part of the Upper Limestone Formation, the Upper Hirst Coal has been widely worked under the Central Coalfield and west Fife. Commonly averaging around 10 ft (3

m) thick, it was the last seam to be worked by deep mining in Scotland at Longannet Colliery, which closed in March 2002 due to flooding.

The overlying **Passage Formation** is approximately 1,250 ft (380 m) thick and of Namurian age. The formation comprises alternating fine- to coarse-grained sandstone and structureless clayrock, with minor siltstone, mudstone, limestone, ironstone, cannel and coal. Marine faunas are diverse at the base, but become progressively impoverished upwards (Browne *et al.* 1999). Abnormally thick coal deposits were excavated opencast in the Westfield Basin (central Fife) from 1955 until 1997 from the Passage Formation and Coal Measures Group.

### 4.4 Scottish Coal Measures Group

The Scottish Coal Measures Group is Westphalian in age and comprises repeated cycles of sandstone, siltstone, mudstone, coal and seatearth, arranged in both upward-fining and upward-coarsening units. A wide range of alluvial and lacustrine environments of deposition is represented including wetland forest and soils (coal and seatrock), floodplain (planty or rooted siltstone and mudstone), river and delta distributary channel (thick sandstones), prograding deltas (upward-coarsening sequences) and shallow lakes (mudstones with non-marine faunas). Marine bands are rare, but provide important stratigraphic markers. Some parts of the Scottish Coal Measures Group contain thick mudstones, but nowhere onshore apart from under the Mauchline Basin in Ayrshire are these buried at depths greater than 3,280 ft (1,000 m) (Monaghan 2013). The group is divided into three formations: the Lower, Middle and Upper Coal Measures that are around 750 ft (230 m), 1,150 ft (350 m) and up to approximately 3,940 ft (1,200 m) thick respectively. Coal seams have historically been extensively worked in the Lower and Middle Coal Measures formations.

### 4.5 Volcanic formations

A palaeogeography for the lower Visean, before the deposition of the Gullane Formation, is provided to illustrate the volcanic rocks on which the prospective shale units were deposited (Figure 3). Volcanism was widespread in the early Visean, most voluminous in the west. An unconformity is recorded in the sedimentary succession during the TS palynomorph zone (Stephenson *et al.* 2004).



Figure 3 Summary of pre-Gullane Formation volcanic activity (c.339 Ma, TS palynomorph zone). a) Evidence from well/borehole and surface exposures. Note that wells/boreholes proving the volcanic rocks or unconformity are surrounded by shading, other wells/boreholes do not prove this interval b) Summary of the palaeogeography. Evidence is patchy and the reconstruction is tentative. Dashed lines are faults and folds likely to have been active.

The volcanism is divided into a number of formations of differing age and rock type.

The **Bathgate Group** of pyroclastic rocks and basaltic lavas comprises three formations of slightly differing ages and distinct locations. The **Bathgate Hills Volcanic Formation** is up to 3,280 ft (1,000 m) thick in the West Lothian to Falkirk area and is interbedded with strata from towards the top of the West Lothian Oil-Shale Formation (Two Foot Coal) to the Passage Formation. The subsurface extent of the formation was estimated using borehole and magnetic data (Cameron *et al.* 1998; main report Figure 32).

In the Saline area of west Fife, tuffs and basalts are included within the Limestone Coal and Upper Limestone formations (BGS DigMap 1:50,000 scale). Read (1988) used the term 'Bo'ness Line' to describe their NNE alignment from Saline to the Bathgate Hills, on the eastern side of the Clackmannan syncline.

The **Kinghorn Volcanic Formation**, up to 1,310-1,640 ft (400-500 m) thick, interdigitates with the upper part of the Sandy Craig Formation, the Pathhead Formation and the basal Lower Limestone Formation to the west of Kinghorn, Fife (main report Figure 32). Volcanic rocks of similar type and age are observed in the Firth of Forth 1 and Milton of Balgonie 1 wells, as well as in former shafts at Seafield Colliery and on Inchkeith island, suggesting a significant eastwards extent of this formation.

The **Salsburgh Volcanic Formation** was previously only identified as being 335 ft (102 m) thick in the Salsburgh 1A well beneath the Burdiehouse Limestone of the West Lothian Oil-Shale Formation (Browne *et al.* 1999). It is interpreted (Appendix C) that volcanism of similar stratigraphic position and character is also present in Salsburgh 2, Leven Seat 1, and possibly West Calder 1 wells, reaching a maximum thickness of 1,974 ft (602 m) in Leven Seat 1. In the Leven Seat 1 well, the age of the volcanism ranges from around the NM/TC palynomorph zone boundary to lower in the Asbian (TC palynomorph zone; Petrachem 1989).

As time-equivalents of key shale-bearing formations, the temporal and spatial extent of these three volcanic formations is critical to the estimation of the shale resource volume.

The Clyde Plateau, Arthur's Seat and Garleton Hills volcanic formations and Charles Hill Volcanic Member are generally stratigraphically below (older than) the shale-bearing units. Integrating radiometric and biostratigraphical ages on a recent timescale (Figure 1) implies that the youngest volcanic rocks (e.g. youngest Clyde Plateau) are likely time equivalent with the oldest Gullane Formation strata (Monaghan *et al.* in press).

In East Lothian, the **Garleton Hills Volcanic Formation** consists of basaltic to trachytic lavas, tuffs and subordinate volcaniclastic sedimentary rocks dated at around 343 Ma (Monaghan & Pringle 2004, Monaghan & Parrish 2006). Away from the outcrop, the formation has been proved as far west as the Spilmersford borehole.

In West Lothian and Edinburgh, the **Arthur's Seat Volcanic Formation** consists of ankaramite to mugearite lavas, tuffs and volcaniclastic sedimentary rocks dated around 341-335 Ma (Monaghan *et al.* in press). Volcanic rocks at the southern end of the Midlothian Syncline (at Carlops) and in Midlothian 1 are interpreted as an eastward extension of this volcanic activity. Palynomorphs indicate an Asbian (TC) age for Gullane Formation strata partially underlying (in Midlothian 1) and strata overlying (Neves *et al.* 1973) the volcanics. Basalts to the south-east of Livingston at Corston Hill are correlated with the Arthur's Seat Volcanic Formation.

Near Aberdour, west Fife and the island of Inchcolm in the Firth of Forth, the basaltic lavas and tuffs of the **Charles Hill Volcanic Member** are interbedded between the Anstruther and Fife Ness formations. These rocks appear to be at a similar stratigraphical level to the uppermost Arthur's Seat Volcanic Formation, or the lowermost Salsburgh Volcanic Formation. Volcanic rocks at this stratigraphic position are seen in Rosyth 1, South Fod 1 and possibly Blackness 1 and Easter Pardovan 1, suggesting that the Charles Hill Volcanic Member has a greater areal extent than previously recognised.

The basalts to rhyolite lavas, tuffs and volcaniclastic sedimentary rocks of the **Clyde Plateau Volcanic Formation**, up to 2,950 ft (900 m) thick, form the high ground to the north, west and south of Glasgow. The southern Clyde Plateau lavas have been dated at around 335-338 Ma (Monaghan & Pringle 2004, Monaghan & Parrish 2006, Monaghan *et al.* in press). Outcrops of volcanic rock correlated to the Clyde Plateau Volcanic Formation also occur at the southern margin of the Central Coalfield (e.g. in the Carnwath area).

Several ash and tuff beds are recognised within the Strathclyde Group; the Crosswood and Seafield-Deans ashes are two of the thickest examples of this extrusive volcanism that persisted through deposition of the West Lothian Oil-Shale Formation.

### 4.6 Intrusive igneous rocks and vents

Intrusive igneous rocks can be largely divided into three groups: (a) Carboniferous alkali basaltic sills, (b) end-Carboniferous sills and dykes, and (c) Permian vents and plugs.

Carboniferous alkali basaltic sills are common in Fife. Evidence from borehole records indicates that the sill morphology was influenced by pre-existing sedimentary basins and growth faults, in that maximum sill thicknesses (approximately 620 ft, 190 m) occur in the deepest parts of the basins and that they become transgressive across the faults (Walker & Francis 1987). Borehole data also indicate a highly complex magma-host sediment interaction that resulted from high-level emplacement into wet sediments (Walker & Francis 1987). Alkaline basaltic sills are also found in the Glasgow area and to the north and west of Edinburgh.

During Late Carboniferous times (Monaghan & Parrish 2006) there was widespread emplacement of the quartz-dolerite Midland Valley Sill-complex and related dykes (Francis 1982). The Midland Valley Sill-complex extends across Central to West Fife, the northern part of the Central Coalfield and West Lothian (Cameron and Stephenson 1985 p. 118) where it has a profound local effect on vitrinite reflectance maturity values (see main report section 3.6). This sill is also thickest, at more than 490 ft (150 m), in the deepest parts of sedimentary basins; the magma was apparently supplied by feeder dykes (Francis 1982). Quartz-dolerite dykes up to 130 ft (40 m) wide cut across strata as young as Westphalian C on roughly east-west trends.

# **5 BGS Lexicon codes used for stratigraphy of interest**

Lexicon code	Name
ABY	Aberlady Formation
AHSH	Abbeyhill Shales
ARBS	Anstruther Formation
ASV	Arthur's Seat Volcanic Formation
BGN	Ballagan Formation
BHV	Bathgate Hills Volcanic Formation
BINS	Binnend Sandstone
BKME	Black Metals Member
BLLS	Blackhall Limestone
BMA	Broxburn Marls
BMMB	Balmore Marine Band
BNSH	Broxburn Shale
BSLS	Barracks Limestone
CDE	Calders Member
CHVO	Charles Hill Volcanic Member
CMSC	Scottish Coal Measures Group
CPV	Clyde Plateau Volcanic Formation
DLUL	Duloch Under Limestone
DTSH	Dunnet Shale
FEL	Fells Limestone
GHV	Garleton Hills Volcanic Formation
GNST	Granton Sandstones
GUL	Gullane Formation
НМА	Houston Marls
HON	Hopetoun Member
HSS	Hailes Sandstone
JSB	Johnstone Shell Bed
KNW	Kinnesswood Formation
KPF	Knox Pulpit Sandstone Formation
LCMS	Scottish Lower Coal Measures Formation
LLGS	Lower Limestone Formation
LSC	Limestone Coal Formation
LWM	Lawmuir Formation
MCMS	Scottish Middle Coal Measures Formation
PDB	Pathhead Formation
PGP	Passage Formation
РМВ	Pittenweem Formation
PMSH	Pumpherston Shales
PNSB	Pumpherston Shell Bed
PRA	Port Edgar Ash
RSH	Raeburn Shale
SALV	Salsburgh Volcanic Formation
SCB	Sandy Craig Formation
ULGS	Upper Limestone Formation
WASH	Wardie Shales Member
WLO	West Lothian Oil-Shale Formation

See <u>www.bgs.ac.uk/Lexicon</u> for more details.

# 6 Equivalence table of previous and current stratigraphical nomenclature

		Lithostratigraphical Units												
Subsystem	Subsystem Series Stage		Formations						Groups		OLD CLASSIFICATIONS			
				Central Coalfield	Ayrshire	Fife	West Lothian East Lothian							
		С	Bolsovian		Upper Coal Measures							UPPER (BARREN) COAL MEASURES		
	Westphalian	в	Duckmantian	Duckmantian Middle Coal Measures						Coa	I Measures	MIDDLE COAL MEASURES	PRODUCTIVE	
	A Langsettian Lower Coal Measures								LOWER COAL MEASURES	COAL MEASURES				
Silesian			Chokierian - Yeadonian		Passage Formation						ckmannan up	PASSAGE GROUP		
	Namurian Arnsbergian				Upper Limestone Formation							UPPER LIMESTONE	GROUP	
			Pendleian	eian Limestone Coal Formation							LIMESTONE COAL GROUP			
					Lower Limestone Formation					Bathgate	LOWER LIMESTONE	GROUP		
			Brigantian	Lawmuir Formati	on	Pathhead Formation	West Lothian Oil Shale		le Abadadu Formation		Group	UPPER OIL SHALE		
			Asbian	Kirkwood Format	ion	Sandy Craig Formation	Formation		Aberlady Formation		GROUP			
	Viséan					Pittenweem Formation							CALCIERDOUS	
Dinantian		Arundian - Holkerian		Clyde Plateau Volcanic Formation		Anstruther Formation		Gullane I Arthur's Seat	Formation Garleton Hills	Strathclyde Group		LOWER OIL SHALE GROUP	CALCIFEROUS SANDSTONE MEASURES	
						Fife Ness Formation		Volcanic Formation	Volcanic Formation					
			Chadian			Clyde Sandstone Format	ion		Dellager Francisco		veluda	CEMENTSTONE		
	Tournaisian		Courcewar			Ballagan Formation			Banagan Formation	Gro	up	GROOP		
		courceyail			Kinnesswood Formation						UPPER OLD RED SANDSTONE (part)			

Figure 4 Summary of current and previous Midland Valley of Scotland stratigraphical nomenclature, from Browne et al. (1999). Some subsequent changes to the timing of volcanic formations have been made as shown in Figure 1.

7 Tables of oil and gas shows

Well name	DECC well registration number	Drilled by	Year drilled	County	Intervals bearing hydrocarbons	Status	Gas shows & testing
Airth 1	LF/27- 2	Hillfarm Coal Company	1993	Clackmannanshire	LSC	2	Coal bed methane
Bargeddie 1	LG/05-1	Marinex Petroleum	1989	Glasgow City	WLO	2	DST: 360 mcf/d, produced 7.3 mmscf before depletion
Blackness 1	LH/03- 2	D'Arcy	1945	West Lothian	WLO	2	DST: "produced 229 cf"
Calais 3	LF/28-6	Berkeley Resources	1986	Fife		0	Detected: 7,000 ppm
Carrington 1	LH/05-25	LASMO	1984	Midlothian		0	Detected: 1,100 ppm
Cousland 1	L33/01-1	D'Arcy	1938	Midlothian	WLO	3	DST: 5.9 mmcf/d; produced 300 mmcf (Hallett <i>et al</i> . 1985)
Cousland 2	LH/05- 5	D'Arcy	1939	Midlothian	WLO	2	DST: 5,000 cf/d
Cousland 3	L33/01-5	D'Arcy	1939	Midlothian		0	No gas shows
Cousland 4	LH/05-14	D'Arcy	1947	Midlothian	WLO, GUL	2	DST: 90 - 101,000 cf/d
Cousland 5	L33/01-7	D'Arcy	1954	Midlothian	WLO	2	DST: 3,850 cf/d
Cousland 6	L33/01-8	B.P.	1959	Midlothian	WLO	2	DST: 150 cf/d
Craighead 1	LH/01- 2	Taylor Woodrow	1982	North Lanarkshire		0	"No significant shows"
D'Arcy 1	LH/05-1	S Pearson	1922	Midlothian	WLO	2	DST: 30,000 cf/d
Duloch 3	LF/29-3	Berkeley Resources	1981	Fife		0	No gas shows
Easter Pardovan 1	LH/03-3	D'Arcy	1946	West Lothian	WLO	2	DST: 13,000 cf/d
Firth of Forth 1	L25/26-1	Conoco	1990	Firth of Forth		0	No gas shows
Inch of Ferryton 1	LF/27- 1	Tricentrol	1986	Clackmannanshire		1	Detected: up to 7%
Kelty Bridge 1	LF/29- 5	Anvil Exp	1984	Perth & Kinross		0	No gas shows
Midlothian 1	LH/05- 2	Anglo-American	1937	Midlothian	GUL	2	DST: 1.4 mmcf/d
Midlothian 2	LH/05-4	Anglo-American	1938	Midlothian		0	Detected: "gas cut mud"
Midlothian 3	LH/05- 9	Anglo-American	1939	Midlothian	WLO	2	DST: 960,000 cf/d
Midlothian 4	LH/05-10	Anglo-American	1939	Midlothian		0	No gas shows
Midlothian 5	LH/05-12	Anglo-American	1939	Midlothian		0	No gas shows
Pumpherston	LH/03-4	B.P.	1962	West Lothian	WLO	2	DST: 7,500 cf/d
Salsburgh 1A	LH/01- 1A	D'Arcy	1944	North Lanarkshire	WLO	2	DST: 330,000 cf/d (Hallett et al. 1985)
Salsburgh 2	LH/01-3	Candecca	1985	North Lanarkshire	LSC	1	Detected: 2% - coal assoc.
Stewart 1	LH/05- 15	LASMO	1981	Midlothian		1	Detected: up to 2%
Straiton 1	LH/05-24	LASMO	1984	Midlothian		0	Detected: up to 1,000 ppm
Straiton 1Z	LH/05- 24Z	LASMO	1984	Midlothian		0	Detected: <100 ppm
West Calder 1	LH/03-1	S Pearson	1919	West Lothian	?WLO	2	DST: 50,000 cu ft

Table 1 List of gas discoveries made in the Midland Valley of Scotland study area. Abbreviations : LSC = Limestone Coal Formation; LLGS = Lower Limestone Formation; WLO = West Lothian Oil-Shale unit; GUL = Gullane unit. Status: 1 = significant gas show (> 1%); 2 = DST which produced gas to surface; 3 = economic gas production.

Well name	DECC well	Drilled by	Year	County	Intervals bearing	Status	Oil shows & testing
	registration		drilled		hydrocarbons		
	number						
Bargeddie 1	LG/05- 1	Marinex Petroleum	1989	Glasgow City		0	No oil shows
Blackness 1	LH/03- 2	D'Arcy	1945	West Lothian	WLO	2	DST: "270 gallons/d "
Calais 3	LF/28- 6	Berkeley Resources	1986	Fife	LLGS, WLO	1	Shows: OCW, fluor.
Carrington 1	LH/05-25	LASMO	1984	Midlothian	LLGS, WLO	2	DST: 4.18 bbl/d, not to surface
Cousland 1	L33/01- 1	D'Arcy	1938	Midlothian	WLO	2	DST: "few gallons" recovered
Cousland 2	LH/05- 5	D'Arcy	1939	Midlothian	WLO	1	Shows: oil in sands
Cousland 3	L33/01- 5	D'Arcy	1939	Midlothian	LLGS, WLO	1	Shows: oil in sands
Cousland 4	LH/05-14	D'Arcy	1947	Midlothian	WLO	2	DST: 0.71 bbl/d
Cousland 5	L33/01- 7	D'Arcy	1954	Midlothian	WLO	2	DST: 0.95 bbl/d
D'Arcy 1	LH/05-1	S. Pearson	1922	Midlothian	WLO	2	DST: 0.85 bbl/d [7 tons in 56 days]
Duloch 3	LF/29- 3	Berkeley Resources	1981	Fife		1	Shows: OCW, flour., staining
Easter Pardovan 1	LH/03-3	D'Arcy	1946	West Lothian	WLO	1	Shows: bitumen residue
Firth of Forth 1	L25/26-1	Conoco	1990	Firth of Forth	WLO	1	Shows: waxy oil recovered
Inch of Ferryton 1	LF/27- 1	Tricentrol	1986	Clackmannanshire	LSC, LLGS	1	Shows: OCW, fluor.
Kelty Bridge 1	LF/29- 5	Anvil Exp	1984	Perth & Kinross		1	Shows: OCW
Lathalmond 1	LF/28-8	Pentex	1990	Fife		1	"Poor shows"
Leven Seat 1	LH/07- 1	Kelt	1988	South Lanarkshire	LLGS, WLO	1	"Both good and poor shows"
Midlothian 1	LH/05-2	Anglo-American	1937	Midlothian		1	Shows: oil in sands
Midlothian 2	LH/05-4	Anglo-American	1938	Midlothian		0	No oil shows
Midlothian 3	LH/05-9	Anglo-American	1939	Midlothian	WLO	3	Produced: "3.5 bbl/day until 1964"
Midlothian 4	LH/05- 10	Anglo-American	1939	Midlothian		0	No oil shows
Midlothian 5	LH/05-12	Anglo-American	1939	Midlothian	WLO	1	Shows: "oil in ditch"
Milton of Balgonie 1	LF/25- 5	Burmah	1984	Fife	LLGS	2	DST: 0.47 bbl/d, waxy oil
Rosyth 1	LF/28- 1	Anglo-American	1940	Fife	WLO	1	"Shows"
Salsburgh 1A	LH/01- 1A	D'Arcy	1944	North Lanarkshire		0	No oil shows
Salsburgh 2	LH/01-3	Candecca	1985	North Lanarkshire		1	Shows: fluor.
Stewart 1	LH/05- 15	LASMO	1981	Midlothian	WLO, GUL	1	Shows: OCW, fluor., staining
Straiton 1	LH/05-24	LASMO	1984	Midlothian	WLO	1	Shows: fluor., OCW, staining
West Calder 1	LH/03-1	S. Pearson	1919	West Lothian		1	"Oil shows"

Table 2 List of oil discoveries made in the Midland Valley of Scotland study area. Abbreviations: LSC = Limestone Coal Formation; LLGS = Lower Limestone Formation; WLO = West Lothian Oil-Shale unit GUL = Gullane unit. Status: 1 = significant oil show; 2 = DST which produced oil to surface; 3 = economic oil production. Shows: fluor = fluorescence; OCW = oil-cut water.

#### References

See main report
# Appendix D Results of BGS 2014 Rock-Eval analysis (C. Vane & V. Moss-Hayes, BGS Keyworth)

Sample ID	Borehole	Depth (m)	Depth (feet)	Unit	Qty (mg)	S1 (mg /g)	S2 mg /g)	PI	Tmax (°C)	TpkS2 (°C)	S3CO (mg/g)	S3'CO (mg/g)	S3 (mg /g)	S3' (mg /g)	PC (%)	RC (%)	ТОС (%)	HI	OICO	OI	pyro MINC (%)	Oxi MINC (%)	MINC (%)
SSK40255	Bargeddie	965	3167	WLO	59.91	0.36	1.92	0.16	445	487	0.02	0.3	0.07	4.9	0.2	2	2.2	87	1	3	0.14	0.08	0.22
SSK40297	Bargeddie	966	3170	WLO	61.15	0.13	0.5	0.21	438	480	2.76	7.2	1.98	159.3	0.38	0.73	1.11	45	249	178	4.5	0.05	4.55
SSK40298	Bargeddie	967	3173	WLO	59.51	0.6	3.97	0.13	436	478	0.07	0.4	0.03	1.9	0.39	3.74	4.13	96	2	1	0.06	0.08	0.14
SSK40299	Bargeddie	968	3177	WLO	64.75	0.07	0.27	0.21	455	497	0.01	0	0	0.7	0.03	0.68	0.71	38	1	0	0.02	0.05	0.07
SSK40256	Salsburgh 2	1055	3462	WLO	63.52	0.82	3.68	0.18	455	497	0.02	0.2	0	1.1	0.38	3.25	3.63	101	1	0	0.03	0.09	0.12
SSK40257	Salsburgh 2	1056	3463	WLO	58.12	0.74	3.76	0.16	455	497	0.02	0.3	0.04	2.2	0.38	2.92	3.3	114	1	1	0.07	0.61	0.68
SSK40261	Stewart 1	495	1625	WLO	63.68	0.14	7.4	0.02	443	485	0.07	0.1	0.08	4.7	0.63	1.51	2.14	346	3	4	0.13	0.03	0.16
SSK40260	Stewart 1	508	1665	GUL	62.22	0.06	0.52	0.11	438	480	0.03	0.1	0.29	5.5	0.06	1.13	1.19	44	3	24	0.15	0.02	0.17
SSK40300	Stewart 1	511	1675	GUL	58.25	0.24	17.16	0.01	446	488	0.14	0.3	0.01	1.3	1.46	2.02	3.48	493	4	0	0.04	0.04	0.08
SSK40259	Stewart 1	819	2687	GUL	64.07	0.37	1.31	0.22	444	486	0.04	0.3	0.07	3.9	0.15	2	2.15	61	2	3	0.11	0.15	0.27
SSK40258	Stewart 1	821	2694	GUL	65.98	0.21	1.03	0.17	440	482	0.04	0.2	0.51	10.5	0.12	1.58	1.7	61	2	30	0.29	0.06	0.35
SSK40263	Airth 6	865	2837	LSC	62.87	0.66	3.62	0.15	450	492	1.69	0.2	0.47	40.5	0.44	3.21	3.65	99	46	13	1.11	0.08	1.19
SSK40301	Airth 6	926	3037	LSC	61.48	2.18	7.83	0.22	442	484	0.17	0.1	0.1	15.1	0.84	4.91	5.75	136	3	2	0.41	0.11	0.52
SSK40262	Airth 6	935	3066	LSC	63.52	1.05	4.7	0.18	428	470	0.33	0.1	0.22	15.9	0.5	3.06	3.56	132	9	6	0.44	0.08	0.52
SSK40264	Craighead 1	871	2856	WLO	60.96	0.44	4.62	0.09	451	493	0.13	0.1	0.75	17.9	0.45	2.1	2.55	181	5	29	0.49	0.04	0.53
SSK40265	Craighead 1	783	2570	WLO	63.85	1.16	14.52	0.07	444	486	0.17	0.5	0.05	0.5	1.32	5.53	6.85	212	2	1	0.02	0.08	0.11
SSK40266	Cousland 6	436	1429	WLO	66.73	0.23	1.41	0.14	436	478	0.19	0.3	1.46	10.4	0.19	2.36	2.55	55	7	57	0.29	0.06	0.35
SSK40267	Cousland 6	582	1908	WLO	59.12	0.07	0.17	0.28	420	462	0.05	0.3	0.36	18	0.04	0.07	0.11	155	45	327	0.5	0.29	0.79
SSK40268	Milton of Balgonie 3	1130	3708	LLGS	60.75	0.92	2.88	0.24	502	544	0.16	0.2	0.09	0.5	0.33	4.11	4.44	65	4	2	0.02	0.08	0.1
SSK40269	Milton of Balgonie 3	1146	3760	LLGS	61.9	0.8	2.81	0.22	491	533	0.08	0.3	0.11	0.5	0.31	3.12	3.43	82	2	3	0.02	0.05	0.07
SSK40270	Milton of Balgonie 3	1184	3884	WLO	65.49	0.69	1.83	0.27	549	591	0.08	0.4	0.04	0.2	0.22	4.65	4.87	38	2	1	0.01	0.08	0.09
SSK40271	Milton of Balgonie 3	1188	3897	WLO	60.95	1.11	7.33	0.13	454	496	0.16	0.5	0.49	8.5	0.73	2.9	3.63	202	4	13	0.24	0.16	0.4
SSK40272	Pumpherston	244	800	GUL	66.91	0.17	0.36	0.32	404	446	0.03	0	0.01	0.9	0.05	0.95	1	36	3	1	0.02	0.17	0.19

SSK40302	Pumpherston	472	1550	GUL	65.12	1.08	3.99	0.21	448	490	0.12	0.1	0.12	4	0.43	2.8	3.23	124	4	4	0.11	0.06	0.17
SSK40273	Pumpherston	756	2480	GUL	58.08	0.25	0.76	0.25	455	497	0.09	0	0.22	23.4	0.09	1.41	1.5	51	6	15	0.64	0.01	0.64
SSK40274	Pumpherston	946	3105	GUL	65.76	0.16	1.11	0.13	455	497	0.04	0.1	0.06	1.7	0.11	1.13	1.24	90	3	5	0.05	0.05	0.09
SSK40303	Pumpherston	1170	3839	GUL	63.82	0.37	1.96	0.16	456	498	0.78	0.2	1.82	40.9	0.28	2.32	2.6	75	30	70	1.12	0.31	1.43
SSK40304	Glenrothes	191	628	WLO	59.8	0.05	0.09	0.34	494	536	0.02	0	0	0	0.01	1.85	1.86	5	1	0	0	0.04	0.04
SSK40275	Glenrothes	194	635	WLO	58.27	0.01	0	0.71	478	520	0.01	0	0	0	0	1.82	1.82	0	1	0	0	0.05	0.05
SSK40276	Glenrothes	224	735	BGN	63.98	0.03	0.19	0.13	594	636	0.09	0	0	4.1	0.02	1.48	1.5	13	6	0	0.11	0.77	0.88
SSK40277	Glenrothes	316	1036	BGN	59.24	0.02	0.08	0.19	456	498	0	0	0	3.6	0.01	0.44	0.45	18	0	0	0.1	1.87	1.97
SSK40353	Glenrothes	317	1040	BGN	63.17	0.08	0.35	0.18	426	468	0.03	0.2	0.09	9	0.04	0.76	0.8	44	4	11	0.25	3.78	4.03
SSK40278	Glenrothes	318	1042	BGN	57.94	0.07	0.12	0.37	496	538	0.04	0	0	2.3	0.02	0.18	0.2	60	20	0	0.06	0.76	0.82
SSK40279	Duloch 3A	112	367	WLO	64.4	0.16	0.29	0.36	567	609	0.06	0	0.12	1.3	0.04	1.35	1.39	21	4	9	0.04	0.02	0.05
SSK40280	Duloch 3A	113	372	WLO	62.87	0.12	0.26	0.32	569	611	0.39	0	0.56	21.7	0.06	0.96	1.02	25	38	55	0.59	0.01	0.6
SSK40281	Duloch 3A	162	531	WLO	60.16	0.09	0.22	0.29	381	423	0.06	0	0	0	0.03	0.26	0.29	76	21	0	0	0.02	0.02
SSK40291	Kelty Bridge	421	1380	WLO	58.86	0.27	0.14	0.66	293	335	0.16	0	0.12	8.4	0.04	1.49	1.53	9	10	8	0.23	0.04	0.27
SSK40292	Kelty Bridge	293	960	WLO	65.77	0.29	0.16	0.65	298	340	0.17	0	0.4	20.6	0.06	1.58	1.64	10	10	24	0.56	0.09	0.65
SSK40293	Kelty Bridge	165	540	WLO	62.29	0.56	2.51	0.18	446	488	1.29	0.3	2.66	43.9	0.39	3.09	3.48	72	37	76	1.2	0.09	1.29
SSK40294	Kelty Bridge	34	110	LLGS	56.03	0.68	3.06	0.18	430	472	0.23	1.2	1.39	31.9	0.38	4.34	4.72	65	5	29	0.9	0.34	1.23
SSK40286	Spilmersford	882	2894	BGN	60.33	0.06	0.08	0.45	333	375	0.03	0.1	0.27	5.9	0.02	0.53	0.55	15	5	49	0.16	0.17	0.33
SSK40287	Spilmersford	879	2883	BGN	65.54	0.02	0.13	0.15	450	492	0.16	0	0.61	21.6	0.04	0.33	0.37	35	43	165	0.59	4.34	4.93
SSK40289	Spilmersford	709	2325	BGN	64.35	0.02	0.12	0.13	437	479	0.04	0.1	0.41	9.6	0.03	0.2	0.23	52	17	178	0.26	0.29	0.55
SSK40288	Spilmersford	155	509	GUL	65.96	0.24	2.79	0.08	431	473	0.2	0.8	0.68	14.6	0.3	2.39	2.69	104	7	25	0.42	2.68	3.1
SSK40290	Spilmersford	142	465	GUL	62.6	0.92	16.52	0.05	428	470	2.94	3.3	3.13	4.2	1.73	15.83	17.56	94	17	18	0.19	0.04	0.23
SSK40296	Levenseat 1	1466	4810	INV	66.2	0.05	0.22	0.19	426	468	0.17	0	1.06	15.1	0.06	0.21	0.27	81	63	393	0.41	1.95	2.36
SSK40282	Lawmuir 1A	46	151	LWM	67.29	0.06	0.54	0.09	440	482	0.08	0.3	0.15	0.6	0.06	2.03	2.09	26	4	7	0.02	0.06	0.08
SSK40283	Lawmuir 1A	71	231	LWM	66.06	0.04	0.25	0.13	438	480	0.25	0	2.74	10.7	0.11	0.65	0.76	33	33	361	0.29	0.03	0.32
SSK40284	Lawmuir 1A	179	586	LWM	65.83	0.07	0.15	0.33	417	459	0.33	0	3.27	10.3	0.12	0.74	0.86	17	38	380	0.28	0.03	0.31
SSK40285	Lawmuir 1A	190	622	LWM	61.14	0.03	0.15	0.18	442	484	0.06	0	0.16	0.8	0.02	0.54	0.56	27	11	29	0.02	0	0.02

Table 1 Raw data from the BGS 2014 Rock-Eval analysis. Stratigraphic codes in the 'unit' column are LSC=Limestone Coal Formation, LLGS=Lower Limestone Formation, WLO=West Lothian Oil-Shale unit, GUL= Gullane unit, LWM= Lawmuir Formation, INV=Inverclyde Group, BGN=Ballagan Formation.

The sampling rationale and locations of samples are discussed in the main report, along with the interpretation of the results. Table 1 above gives the raw data.

# Appendix E Mineralogical analysis of Carboniferous fine-grained sedimentary rocks from the Midland Valley of Scotland

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# Summary

This report presents the results of a mineralogical study carried out on a suite of 50 samples of Carboniferous fine-grained sedimentary rock samples collected from boreholes located in the Midland Valley of Scotland. The samples were collected from the Bargeddie 1, Salsburgh 2, Stewart 1, Airth 6, Craighead 1, Cousland 6, Milton of Balgonie 3, Pumpherston 1, Glenrothes, Duloch 3, Duloch 3A, Kelty Bridge 1, Spilmersford, Leven Seat 1 and Lawmuir 1A boreholes.

The study was commissioned by the Department of Energy & Climate Change (DECC) as part of an assessment of potential for unconventional gas and oil exploration in the area.

Mineralogical analysis was carried out using a combination of whole-rock powder and <2  $\mu$ m clay mineral X-ray diffraction (XRD) techniques.

Whole-rock powder XRD analyses reveal that the samples are composed of variable proportions of quartz, feldspar (plagioclase and K-feldspar), carbonates (calcite, dolomite, ankerite/Fe-dolomite and siderite), clay minerals/phyllosilicates ('mica', kaolinite and chlorite), pyrite and jarosite. An average composition for the samples would be ~59% phyllosilicates/clay minerals, ~9% carbonate minerals and ~32% QFP (quartz, feldspar and pyrite).

Less than 2 µm clay mineral assemblages are generally composed of various amounts of illite, illite/smectite (I/S), kaolinite and an intermediate Fe/Mg chlorite. Minor proportions of talc were also identified in a few samples. Various I/S compositions were identified. Most samples contain an *R*1-ordered I/S (~85% illite) with a more evolved *R*3-ordered I/S (~92% illite) identified in many of the deeper samples. A less mature *R*1-ordered, ~55% illite I/S was identified in a few samples. Moderately crystalline kaolinite typically forms a major component and intermediate Fe/Mg chlorite a minor component of the clay mineral assemblages. Kaolinite and chlorite can form a more significant component and the latter can become more Mg-rich in some boreholes. An interlayered chlorite/serpentine was identified in a few samples.

The results obtained from this study are broadly in-line with previous peer-reviewed published and commercial analyses. However, the mineralogical compositions of the Midland Valley of Scotland samples are considerably more clay mineral-rich and carbonate-poor than USA unconventional gas-producing shales. In the USA, explorationists target shales with low proportions of clay minerals (generally less than 50%) to allow successful fracture stimulation.

The clay mineral-rich nature of the Midland Valley samples produces a simplistic, mean 'Brittleness Index' (*BI*) value of 0.39.

Clay mineral maturity suggests that the majority of the samples have been buried to ~6 km at 'normal' geothermal gradients (~25°C/km) and probably represent the Light Oil/Wet gas maturity zones. These samples are likely to show a bedding parallel microfabric. The *R*3-ordered I/S (~92% illite) present in fewer samples places these in the Wet Gas/Dry Gas transition zone, equivalent to burial of perhaps 8 km at normal geothermal gradients. Such burial typically produces a bedding-parallel microfabric. The presence of an *R*1, 55% illite I/S in a few samples would seem to suggest shallower burial. However, other evidence suggests that the presence of this I/S is more likely to represent either a greater, initial volcanogenic component to the shale or that these rocks have undergone diagenetic or hydrothermal retrogression.

# **1** Introduction

This report presents the results of mineralogical analyses carried out on a suite of 50 Carboniferous finegrained sedimentary rock samples collected from boreholes located in the Midland Valley of Scotland. The samples were collected from the Bargeddie 1, Salsburgh 2, Stewart 1, Airth 6, Craighead 1, Cousland 6, Milton of Balgonie 3, Pumpherston 1, Glenrothes, Duloch 3, Duloch 3A, Kelty Bridge 1, Spilmersford, Leven Seat 1 and Lawmuir 1A boreholes (see Figure 41 main report). The study was commissioned by the Department of Energy & Climate Change (DECC) as part of an assessment of potential for unconventional gas exploration in the area.

Mineralogical analysis was carried out using a combination of whole-rock powder and <2  $\mu$ m clay mineral X-ray diffraction (XRD) techniques. The samples were also analysed using organic geochemical techniques (RockEval, total organic carbon 'TOC'), the results of which are reported separately. Full sample details, including TOC (%) are shown in Table 1. Table 4 of the main report should be consulted for the stratigraphic context of the formation/unit names referred to in this report.

# 2 Laboratory methods

## 2.1 Initial sample preparation

As indicated in Table 1, the submitted sample batch was variously composed of drill cuttings and fragments of core. Similarly the masses submitted for each sample varied between ~5 and ~20 g, depending on the borehole and material availability.

The submitted samples were initially prepared in the BGS Sample Preparation Facility. Core chips were jawcrushed or crushed in a pestle and mortar to produce a ~2 mm diameter crushate. Half of the crushate was then representatively separated using the cone-and-quarter technique and ball-milled for powder whole-rock XRD analysis [and RockEval and TOC analyses reported elsewhere]. The remaining crushate was used for clay mineral XRD analysis.

### 2.1.1 Whole-rock analysis

In order to provide a finer and uniform particle-size for powder XRD analysis, a 4.5 g portion of the milled sample was micronised under deionised water for 10 minutes with 10% (0.5 g) corundum (American Elements - PN:AL-OY-03-P). The addition of an internal standard allows the validation of quantification results and also the detection of any amorphous species present in the sample. Corundum was selected as its principle XRD peaks are suitably remote from those produced by most of the phases present in the samples and its mass absorption coefficient is similar to the sample matrix.

All corundum-spiked samples were then spray-dried following the method and apparatus described by Hillier (1999). The spray-dried materials were then front-loaded into standard stainless steel sample holders for analysis.

Table 1. Sample list

Borehole	Depth (m)	Depth (ft.)	Sample no.	Stratigraphy	Sample	TOC (%)
	005.2	2167	66840255		type	2.20
	965.3	3167	SSK40255	Mast lathing Oil Shala For	core	2.20
Bargeddie 1	966.2	3170	SSK40297	(WLO)	core	1.11
	967.0	3172.5	SSK40298	(WEO)	core	4.13
	908.3	31/0./5	55K40299		core	0.71
Salsburgh 2	1055.1	3461.75	SSK40256	West Lothian Oil-Shale Fm.	core	3.63
	1055.6	3463.33	SSK40257		core	3.30
	495.2	1624.7	SSK40261	West Lothian Oil-Shale Fm.	core	2.14
	507.5	1665.0	SSK40260	-	core	1.19
Stewart 1	510.6	1675.2	SSK40300	Gullane Fm. (GUL)	core	3.48
	818.94	2686.8	SSK40259	4	core	2.15
	821	2693.6	SSK40258		core	1.70
	864.6	2836.5	SSK40263	Black Metals Marine Band	core	3.65
Airth 6	925.6	3036.75	SSK40301	(BKME), Limestone Coal Fm.	core	5.75
	934.5	3066	SSK40262	(LSC)	core	3.56
Craighead 1	783.3	2570	SSK40265	West Lothian Oil-Shale Fm	core	6.85
eraigheau 1	870.5	2856	SSK40264		core	2.55
Cousland 6	435.6	1429	SSK40266	West Lothian Oil-Shale Fm	core	2.55
Cousiana o	581.6	1908	SSK40267	West Lotinun on Shule Fill.	core	0.11
	1130.2	3708	SSK40268	Lower Limestone Em. (LLGS)	core	4.44
Milton of	1146.0	3760	SSK40269	Lower Linestone I III. (LLGS)	core	3.43
Balgonie 3	1183.7	3883.5	SSK40270	Pathhead Formation (PDB) just	core	4.87
	1187.8	3897	SSK40271	beneath Hurlet Limestone (HUR)	core	3.63
	243.8	800	SSK40272		core	1.00
	472.4	1550	SSK40302		core	3.23
Pumpherston 1	755.9	2480	SSK40273	Gullane Fm.	core	1.50
-	946.3	3104.5	SSK40274	1	core	1.24
	1170.1	3839	SSK40303	1	core	2.60
	191.46	628.1	SSK40304		core	1.86
	193.6	635.2	SSK40275	Pathhead Formation	core	1.82
	223.9	734.6	SSK40276		core	1.50
Glenrothes	315.8	1036.1	SSK40277		core	0.45
	316.95	1039.9	SSK40353	Ballagan Fm. (BGN)	core	0.80
	317.7	1042.3	SSK40278	]	core	0.20
	111.75	366.6	SSK40279		core	1.39
Duloch 3	113.3	371.7	SSK40280	West Lothian Oil-Shale Fm.	core	1.02
Duloch 3A	161.7	530.5	SSK40281	West Lothian Oil-Shale Fm.	core	0.29
	33.5	110	SSK40294	Lower Limestone Fm.	cuttings	4.72
	164.6	540	SSK40293		cuttings	3.48
Kelty Bridge 1	292.6	960	SSK40292	West Lothian Oil-Shale Fm.	cuttings	1.64
	420.6	1380	SSK40291		cuttings	1.53
	141.7	465	SSK40290		core	17.56
	155.1	509	SSK40288	Gullane Fm.	core	2.69
Spilmersford	708.8	2325.3	SSK40289		core	0.23
	878.6	2882.5	SSK40287	Ballagan Fm.	core	0.37
	882.2	2894.4	SSK40286		core	0.55
Leven Seat 1	1466.1	4810	SSK40296	Invercivde Group (INV)	cuttings	0.27
	45 92	150 7	SSK40282		COLE	2 09
Lawmuir 1A	70 5	231 3	SSK40282	1	core	0.76
	178.68	586.2	SSK40284	Lawmuir Fm. (LWM)	core	0.86
	189.6	622.0	SSK40285	1	core	0.56

### 2.1.2 Carbonate removal

Initial inspection of the whole-rock XRD traces suggested that 28 of the 50 samples contained significant proportions of various carbonate minerals (calcite, dolomite and siderite). Since such carbonate species may 'lock-up' clay minerals and prevent their release during size-separation prior to clay mineral XRD analysis, a buffered acid pre-treatment was employed to remove the carbonate species from these samples.

For this, crushed core/cuttings were placed in a 500 ml beaker with ~250 ml of buffered sodium acetate/acetic acid (pH 5.3) and the suspension was treated with ultrasound for 3 minutes. The beakers were then placed in a water bath maintained at 60°C for 6 hours and stirred every hour. The suspensions were then treated to further ultrasound for 3 minutes and left to stand overnight. Next morning the supernatant liquid was discarded. The leaching procedure was then repeated a second time before the material was transferred to a centrifuge bottle and washed three times with distilled water. Where large proportions of siderite were detected (Bargeddie 1, 3170 ft), the leaching procedure was repeated four times.

### 2.1.3 <2 μm fraction clay mineral analysis

To separate a fine fraction for clay mineral XRD analysis, the carbonate-free residue prepared in section 2.1.2 or <2 mm crushate were dispersed in distilled water using a reciprocal shaker combined with ultrasound treatment. The suspension was then sieved on 63  $\mu$ m and the <63  $\mu$ m material placed in a measuring cylinder and allowed to stand. In order to prevent flocculation of the clay crystals, 1 ml of 0.1M 'Calgon' (sodium hexametaphosphate) was added to each suspension. After a time period determined from Stokes' Law, a nominal <2  $\mu$ m fraction was removed and dried at 55°C. 100 mg of the <2  $\mu$ m material was then re-suspended in a minimum of distilled water and pipetted onto a ceramic tile in a vacuum apparatus to produce an oriented mount. The mounts were Ca-saturated using 0.1M CaCl<sub>2</sub>.6H<sub>2</sub>O solution, washed twice to remove excess reagent and allowed to air-dry overnight.

## 2.2 X-ray diffraction analysis

XRD analysis was carried out using a PANalytical X'Pert Pro series diffractometer equipped with a cobalttarget tube, X'Celerator detector and operated at 45kV and 40mA.

The micronised powder samples were scanned from 4.5-85°20 at 2.76°20/minute. Diffraction data were initially analysed using PANalytical X'Pert HighScore Plus version 2.2e software coupled to the latest version of the International Centre for Diffraction Data (ICDD) database.

Following identification of the mineral species present in the sample, mineral quantification was achieved using the Rietveld refinement technique (e.g. Snyder & Bish 1989) using PANalytical HighScore Plus software. This method avoids the need to produce synthetic mixtures and involves the least squares fitting of measured to calculated XRD profiles using a crystal structure databank. Errors for the quoted mineral concentrations are typically  $\pm 2.5\%$ . Where a phase was detected but its concentration was indicated to be below 0.5%, it is assigned a value of <0.5%, since the error associated with quantification at such low levels becomes too large.

The <2 µm oriented mounts were scanned from 2-40°20 at 1.02°20/minute after air-drying, after glycolsolvation, after heating to 375°C for 2 hours and after heating to 550°C for 2 hours. In order to gain further information about the nature of the clay minerals present in the sample, modelling of the <2 µm glycol-solvated XRD profiles was carried out using Newmod-for-Windows™ (Reynolds & Reynolds 1996) software. Modelling was also used to assess the relative proportions of clay minerals present in the <2 µm fraction by comparison of sample XRD traces with Newmod-for-Windows™ modelled profiles. The modelling process requires the input of diffractometer, scan parameters and a quartz intensity factor (instrumental conditions), and the selection of different sheet compositions and chemistries. In addition, an estimate of the crystallite size distribution of the species may be determined by comparing peak profiles of calculated diffraction profiles with experimental data. By modelling the individual clay mineral species in this way, mineral reference intensities were established and used for quantitative standardization following the method outlined in Moore & Reynolds (1997).

# **3 Results**

The results of quantitative powder and <2  $\mu$ m clay mineral XRD analyses are summarised in Tables 2 to 5. Example labelled XRD traces are shown in Figures 1 and 5-9.

## 3.1 Whole-rock analysis

Powder whole-rock XRD analysis indicates that the samples are composed of variable mineralogical assemblages comprising quartz, feldspar (plagioclase and K-feldspar), carbonates (calcite, dolomite, ankerite/Fe-dolomite and siderite), clay minerals/phyllosilicates ('mica', kaolinite and chlorite), pyrite and jarosite (Tables 2 and 3). The term 'mica' indicates the presence of undifferentiated mica species possibly including muscovite, biotite, illite and illite/smectite.

An example whole-rock XRD trace compared to its component mineral standard patterns is shown in Figure 1.

Note that although two forms of siderite were identified in the samples (siderite and a Mn-siderite), these are not differentiated in Tables 2 and 3 and a total siderite content is shown. Similarly ferroan dolomite and ankerite contents are not differentiated and a total content is shown in Tables 2 and 3.

An average composition for the samples would be composed of ~59% clay minerals/phyllosilicates, ~9% carbonate, ~30% quartz ~1% feldspar and ~1% pyrite. However, as shown in the triplot (Figure 2), the assemblages show considerable variation in their compositions e.g. total quartz, feldspar, pyrite (QFP, <0.5 to 72%), total carbonate (not detected to 78%) and total clay minerals/phyllosilicate (~12 to 99%).

Further triplots discriminating the mineralogy of the Midland Valley samples on the basis of borehole and stratigraphy are shown in Figures 3 and 4.

The borehole-grouped data emphasises the considerable variation in the mineralogy of samples collected from the same borehole, perhaps with the exception of the QFP-rich samples in the Salsburgh 2 borehole (Figure 3).

The stratigraphically-grouped triplot (Figure 4) reveals some interesting trends in the mineralogical data. The West Lothian Oil Shale Formation and its lateral equivalents, the Pathhead and Lawmuir formations are generally carbonate-poor, with the exception of the siderite-rich ironstone from Bargeddie 1, 3170 ft. The same West Lothian Oil Shale, Pathhead and Lawmuir formation samples are typically phyllosilicate/clay mineral-rich, particularly some of the samples from the Lawmuir Formation. The most QFP-rich samples are also from the West Lothian Oil Shale Formation. The Ballagan Formation samples are relatively carbonate-rich (calcite) while the samples from the Gullane Formation are relatively phyllosilicate/clay mineral-rich. The few samples from the Black Metals Marine Band within the Limestone Coal Formation present a relatively consistent mineralogy (~67% clay, ~13% carbonate, ~20% QFP).

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Table 2. Summary of quantitative whole-rock XRD analysis (Bargeddie 1, Salsburgh 2, Stewart 1, Airth 6, Craighead 1, Cousland 6, Milton of Balgonie 3 and Pumpherston 1 boreholes)

									Minera	logy (%)					
Barahala	Depth	Comula No.	*Strat-		Silicates		Phyllosil	icates/clay	minerals		Carbo	onates		Sulphi	des etc
Borenoie	(ft.)	Sample No.	igraphy	quartz	plag.	K-feld.	'mica'	kaolinite	chlorite	calcite	dolomite	ankerite/ Fe-dol.	siderite	pyrite	jarosite
	3167	SSK40255		29.2	nd	nd	48.1	20.1	nd	nd	nd	nd	nd	2.7	nd
Dargaddia 1	3170	SSK40297	WI O	9.9	nd	nd	11.8	<0.5	nd	nd	nd	nd	77.7	0.6	nd
Bargeddie 1	3172.5	SSK40298	WLO	21.3	nd	nd	23.5	20.5	0.8	nd	nd	nd	0.6	33.3	nd
	3176.75	SSK40299		39.8	nd	nd	31.7	28.3	nd	nd	nd	nd	<0.5	nd	nd
Calaburah 2	3461.75	SSK40256	W/L O	65.1	4.5	nd	8.3	8.0	11.8	<0.5	nd	nd	nd	1.9	nd
Salsburgh 2	3463.33	SSK40257	WLO	59.6	3.5	nd	24.6	3.5	4.0	4.7	nd	nd	nd	<0.5	nd
	1624.7	SSK40261	WLO	41.2	nd	nd	46.2	10.1	1.8	nd	nd	nd	0.7	nd	nd
	1665.0	SSK40260		30.7	nd	nd	60.4	4.9	2.2	nd	nd	nd	1.8	nd	nd
Stewart 1	1675.2	SSK40300		36.6	nd	nd	50.0	10.3	3.0	nd	nd	nd	nd	nd	nd
	2686.8	SSK40259	GUL	46.0	nd	nd	42.2	7.4	3.2	nd	1.2	nd	nd	nd	nd
	2693.6	SSK40258		31.6	nd	nd	57.0	6.4	3.7	nd	<0.5	nd	1.1	nd	nd
	2836.5	SSK40263	DVA	24.8	nd	nd	46.6	10.2	2.0	nd	nd	nd	16.4	nd	nd
Airth 6	3036.75	SSK40301	BKIME	23.1	nd	nd	39.5	27.7	1.0	nd	nd	nd	8.7	nd	nd
	3066	SSK40262	LJC	10.9	nd	nd	42.5	28.5	3.6	nd	nd	nd	14.5	nd	nd
Craighood 1	2570	SSK40265	WI O	4.2	nd	nd	73.9	19.6	2.2	nd	nd	nd	nd	nd	nd
Craignead 1	2856	SSK40264	WLO	21.7	nd	nd	58.8	6.4	1.9	nd	nd	nd	11.2	nd	nd
Coursland 6	1429	SSK40266	WIO	37.2	nd	<0.5	40.6	17.3	2.9	nd	nd	nd	1.8	nd	nd
Cousiand 6	1908	SSK40267	WLO	52.1	nd	<0.5	34.0	6.9	nd	2.2	nd	nd	2.6	nd	nd
	3708	SSK40268		38.5	nd	nd	44.2	17.3	nd	nd	nd	nd	nd	nd	nd
Milton of	3760	SSK40269	LLGS	52.8	nd	nd	32.4	14.8	nd	nd	nd	nd	nd	nd	nd
Balgonie 3	3883.5	SSK40270	PDB,	45.5	nd	nd	40.7	13.8	nd	nd	nd	nd	nd	nd	nd
	3897	SSK40271	HUR	24.7	nd	nd	52.1	19.0	nd	2.4	nd	nd	<0.5	1.7	nd
	800	SSK40272		27.4	2.2	nd	54.1	8.0	8.1	<0.5	nd	nd	nd	nd	nd
	1550	SSK40302		32.6	nd	nd	55.6	8.7	2.9	nd	nd	nd	nd	<0.5	nd
Pumpherston	2480	SSK40273	GUL	22.7	1.1	nd	63.7	2.0	nd	<0.5	nd	nd	10.4	nd	nd
1	3104.5	SSK40274		22.0	1.0	nd	66.6	7.0	2.8	0.7	nd	nd	nd	nd	nd
	3839	SSK40303		27.0	nd	nd	47.8	2.4	nd	4.1	nd	nd	15.8	0.6	nd

Table 3. Summary of quantitative whole-rock XRD analysis (Glenrothes, Duloch 3, Duloch 3A, Kelty Bridge 1, Spilmersford, Leven Seat 1 and Lawmuir 1A boreholes)

				-					Mi	ineralogy	(%)					
	Depth		*Strat-		Silicates		Phy	llosilicates	/clay mine	erals		Carbo	onates		Sulphi	des etc
Borehole	(ft.)	Sample No.	igraphy	quartz	plag.	K-feld.	'mica'	kaolinite	chlorite	talc	calcite	dolomite	ankerite /Fe-dol.	siderite	pyrite	jarosite
	628.1	SSK40304	חטם	21.8	nd	nd	46.5	26.0	5.0	0.7	nd	nd	nd	nd	nd	nd
	635.2	SSK40275	PDB	32.0	nd	nd	63.4	2.6	0.8	0.6	<0.5	nd	nd	nd	0.7	nd
Clanrathas	734.6	SSK40276		22.9	nd	nd	61.5	2.5	5.1	nd	8.0	nd	nd	nd	nd	nd
Gienrothes	1036.1	SSK40277	PCN	25.7	nd	1.0	52.9	nd	0.9	nd	19.5	nd	nd	nd	nd	nd
	1039.9	SSK40353	DGIN	19.2	nd	nd	37.3	<0.5	1.6	nd	40.7	nd	0.9	nd	<0.5	nd
	1042.3	SSK40278		38.1	nd	2.8	47.7	1.3	0.8	nd	9.0	nd	<0.5	nd	nd	nd
Dulesh 2	366.6	SSK40279		31.4	nd	nd	51.7	14.9	1.9	nd	nd	nd	nd	<0.5	nd	nd
Duloch 3	371.7	SSK40280	WLO	50.0	nd	nd	22.7	17.7	5.8	nd	nd	nd	nd	3.8	nd	nd
Duloch 3A	530.5	SSK40281	WLO	45.7	nd	nd	52.2	1.1	1.0	nd	nd	nd	nd	nd	nd	nd
	110	SSK40294	LLGS	36.5	nd	<0.5	35.8	11.6	nd	nd	nd	nd	4.6	9.4	1.8	nd
Kalta Dalalas (	540	SSK40293		15.3	nd	nd	45.7	22.2	nd	nd	nd	nd	nd	16.8	nd	nd
Keity Bridge 1	960	SSK40292	WLO	70.0	nd	nd	20.1	2.8	nd	<0.5	nd	nd	2.4	1.9	1.8	0.6
	1380	SSK40291		40.9	nd	nd	46.2	6.7	nd	0.6	nd	nd	nd	0.6	5.1	nd
	465	SSK40290		14.5	nd	nd	67.7	16.8	<0.5	nd	nd	nd	nd	nd	nd	0.7
	509	SSK40288	GUL	30.1	nd	nd	32.0	9.7	nd	nd	9.9	nd	16.3	nd	1.9	nd
Spilmersford	2325.3	SSK40289		12.8	nd	nd	81.9	nd	<0.5	nd	5.1	nd	nd	nd	nd	nd
	2882.5	SSK40287	BGN	10.6	nd	nd	41.8	nd	nd	nd	47.4	nd	<0.5	nd	nd	nd
	2894.4	SSK40286		16.8	nd	nd	79.2	nd	1.0	nd	3.0	nd	nd	nd	nd	nd
Leven Seat 1	4810	SSK40296	INV	31.2	12.4	nd	17.7	nd	nd	nd	1.4	36.4	nd	nd	nd	nd
	150.7	SSK40282		4.8	nd	nd	6.1	89.1	nd	nd	nd	nd	nd	nd	nd	nd
	231.3	SSK40283		26.4	nd	nd	27.5	34.1	nd	nd	nd	nd	nd	12.0	nd	nd
Lawmuir 1A	586.2	SSK40284	LVVIVI	28.4	nd	nd	36.5	29.2	nd	nd	nd	nd	nd	6.0	nd	nd
	622.0	SSK40285		<0.5	nd	nd	81.5	18.4	nd	nd	nd	nd	nd	nd	nd	nd

<u>KEY</u> 'mica' undifferentiated mica species including muscovite, biotite, illite and illite/smectite etc

not detected nd

\* see Table 1 for full stratigraphical nomenclature



*Figure 1. Example whole-rock XRD trace (above) compared to extracted peak data (orange sticks, below) and identified component mineral phases as ICDD standard stick patterns (below), sample Stewart 1, 2693.6 ft.* 

APPENDIX E TO THE CARBONIFEROUS SHALES OF THE MIDLAND VALLEY OF SCOTLAND: GEOLOGY AND RESOURCE ESTIMATION



Figure 2. Triplot to illustrate the whole-rock mineralogy of all Midland Valley of Scotland samples.



Figure 3. Triplot of whole-rock mineralogy discriminated on a borehole basis



Figure 4. Triplot of whole-rock mineralogy discriminated on a stratigraphic basis. The Pathhead and Lawmuir formations are within the West Lothian Oil-Shale unit defined in the main report, and the Gullane Fm is part of the Gullane unit.

## 3.2 <2 μm fraction clay mineral analysis

Less than 2  $\mu$ m clay mineral XRD analyses indicate that the clay mineral assemblages of the samples are generally composed of various amounts of illite, illite/smectite, kaolinite and chlorite (Tables 4 and 5). Minor proportions of talc were also identified in a few samples (Glenrothes, 628.1 and 635.2 ft, Kelty Bridge 1, 960 and 1380 ft).

The generated XRD traces are complex and difficult to interpret, even using state-of-the-art modelling packages. However, modelling individual clay species and then combining these to profile-fit the sample traces produced excellent composite matches of background together with peak positions, heights and widths. To illustrate the efficacy of the modelling approach, an example of a NEWMOD II-modelled profile is shown matched to an experimental ethylene glycol-solvated XRD trace in Figure 5.

Table 4. Summary of the relative proportions of clay minerals in the <2  $\mu$ m fractions (Bargeddie 1, Salsburgh 2, Stewart 1, Airth 6, Craighead 1, Cousland 6, Milton of Balgonie 3 and Pumpherston 1 boreholes)

				c	lay mine	ralogy (%	6)		
Borehole	Depth (ft)	Sample no.	⁺Strat- igraphy	illite	illite/ smectite	kaolinite	chlorite	Illite/smectite species	Non-clay minerals
	3167	SSK40255		22	29	49	nd	85%I <i>, R</i> 1	qtz, plag, sid
Dargaddia 1	3170	SSK40297	WI 0	16	21	64	nd	85%I <i>, R</i> 1	qtz, plag, sid
Bargeoule 1	3172.5	SSK40298	WLO	8	12	80	nd	85%I <i>, R</i> 1	qtz, plag, pyrite
	3176.7	SSK40299		13	17	70	nd	85%I <i>, R</i> 1	qtz, plag
Calchurgh 2	3461.7	SSK40256	WI 0	25	22	14	40	85%I <i>, R</i> 1	qtz, plag
Saisburgh 2	3463.3	SSK40257	WLO	32	28	14	26	85%I <i>, R</i> 1	<mark>qtz</mark> , plag
	1624.7	SSK40261	WLO	23	32	32	12	85%I, <i>R</i> 1	qtz, plag
Stewart 1	1665.0	SSK40260		21	31	37	12	85%I <i>, R</i> 1	qtz, plag
	1675.2	SSK40300		27	31	32	10	85%I <i>, R</i> 1	qtz, plag
	2686.8	SSK40259	GOL	34	22	35	9	92%I, <i>R</i> 3	qtz, plag
	2693.6	SSK40258	]	31	31	27	11	92%I <i>, R</i> 3	qtz, plag
	2836.5	SSK40263		22	23	50	5	92%I, <i>R</i> 3	qtz, plag, sid
Airth 6	3036.7	SSK40301	BKIME,L	15	17	62	5	92%I <i>, R</i> 3	qtz, plag
	3066	SSK40262	50	12	10	71	6	92%I <i>, R</i> 3	qtz, plag
Creichead 1	2570	SSK40265	<b>W</b> (10)	18	35	43	5	85%I <i>, R</i> 1	qtz, plag
Craignead 1	2856	SSK40264	WLO	20	42	29	8	70%I <i>, R</i> 0	qtz, plag
Coursland C	1429	SSK40266	WIO	19	23	49	9	85%I, <i>R</i> 1	qtz, plag
Cousianu b	1908	SSK40267	WLO	18	48	28	6	80%I <i>, R</i> 1	qtz, plag
	3708	SSK40268		25	18	57	nd	92%I, <i>R</i> 3	qtz, plag
Milton of	3760	SSK40269	LLGS	22	21	57	nd	92%I, <i>R</i> 3	qtz, plag
Balgonie 3	3883.5	SSK40270	PDB,	21	19	60	nd	92%I, <i>R</i> 3	qtz, plag
	3897	SSK40271	HUR	23	22	48	7	85%I, <i>R</i> 1	qtz, plag
Duranharatan	800	SSK40272		90	nd	nd	10	na	qtz, plag
	1550	SSK40302	]	22	37	34	7	85%I <i>, R</i> 1	qtz, plag
Pumpnerston	2480	SSK40273	GUL	45	40	15	nd	85%I, <i>R</i> 1	qtz, plag
1	3104.5	SSK40274	]	46	26	21	7	85%I, <i>R</i> 1	qtz, plag
	3839	SSK40303		42	26	22	11	85%I, <i>R</i> 1	gtz, plag

KEY

nd not detected

na not applicable

qtz quartz

plag plagioclase feldspar

sid siderite

red text indicates elevated concentrations

+ see Table 1 for full stratigraphical names

Table 5. Summary of the relative proportions of clay minerals in the <2  $\mu$ m fractions (Glenrothes, Duloch 3, Duloch 3A, Kelty Bridge 1, Spilmersford, Leven Seat 1 and Lawmuir 1A boreholes)

					Clay r	nineralo	gy (%)			
Borehole	Depth (ft)	Sample no.	⁺Strat- igraphy	illite	illite/ smectite	kaolinite	chlorite	talc	Illite/smectite species	Non-clay minerals
	628.1	SSK40304	חטט	51	10	nd	26	12	55%I <i>, R</i> 1	qtz, plag
	635.2	SSK40275	PDB	61	19	nd	14	6	55%I <i>, R</i> 1	qtz, plag
Claurathas	734.6	SSK40276		50	27	nd	23	nd	90%I <i>, R</i> 1	qtz, plag
Gienrotnes	1036.1	SSK40277	DCN	69	23	3	5	nd	92%I <i>, R</i> 3	qtz
Duloch 3	1039.9	SSK40353	BGIN	54	35	4	6	nd	92%I, <i>R</i> 3	qtz
	1042.3	SSK40278		63	25	5	6	nd	92%I, <i>R</i> 3	qtz
	366.6	SSK40279		31	22	33	15	nd	62%I, <i>R</i> 1	qtz, plag
Duloch 3	371.7	SSK40280	WLO	15	35	29	20	nd	62%I, <i>R</i> 1	qtz
Duloch 3A	530.5	SSK40281	WLO	24	66	nd	10	nd	62%I, <i>R</i> 1	qtz
	110	SSK40294	LLGS	35	17	49	nd	nd	85%I <i>, R</i> 1	qtz, plag
Kelty Bridge	540	SSK40293		25	8	67	nd	nd	85%I <i>, R</i> 1	qtz, plag
1	960	SSK40292	WLO	64	10	19	nd	6	55%I <i>, R</i> 1	qtz, plag
	1380	SSK40291		63	10	22	nd	5	55%I <i>, R</i> 1	qtz, plag
	465	SSK40290	CUI	24	11	64	nd	nd	85%I <i>, R</i> 1	qtz, plag
Cuilus and	509	SSK40288	GUL	34	20	47	nd	nd	85%I <i>, R</i> 1	qtz, plag
Splimers-	2325.3	SSK40289		72	28	nd	nd	nd	92%I <i>, R</i> 3	qtz
loru	2882.5	SSK40287	BGN	54	43	4	nd	nd	92%I, <i>R</i> 3	qtz, calc
	2894.4	SSK40286		37	60	3	nd	nd	92%I <i>, R</i> 3	qtz
Leven Seat 1	4810	SSK40296	INV	40	51	2	6	nd	92%I, <i>R</i> 3	qtz, plag
Lawmuir 1A	150.7	SSK40282		7	4	90	nd	nd	85%I <i>, R</i> 1	qtz, plag
	231.3	SSK40283	114/54	10	5	85	nd	nd	85%I, <i>R</i> 1	qtz, plag
	586.2	SSK40284		16	8	76	nd	nd	85%I <i>, R</i> 1	qtz, plag
	622.0	SSK40285		14	22	65	nd	nd	92%I, <i>R</i> 3	qtz, plag

 KEY

 nd
 not detected

 qtz
 quartz

 plag
 plagioclase feldspar

 calc
 calcite

 + see Table 1 for full stratigraphical names

### 3.2.1 Illite

Illite was identified in all the separated <2  $\mu$ m fractions by its characteristic air-dry spacings of ~9.98, 4.98 and 3.32Å which remain invariant after glycol-solvation and heating. Newmod II<sup>TM</sup>-modelling of the widths of the illite XRD peaks suggests a typical crystallite-size distribution has a mean defect-free distance of 10 layers (10Å units) and a size range between 1 and 30 layers. Generally the illites appear to have low Fe and high K chemistries with average compositions of ~0.1 Fe and ~0.96 K per (Si, Al)<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>.



Figure 5. Example comparison of Newmod II<sup>m</sup>-modelled and experimental ethylene glycol-solvated XRD trace, sample Spilmersford 509 ft. Horizontal axis,  $^{\circ}2\theta$  Co-K $\alpha$ ; vertical axis, intensity (cps).

#### 3.2.2 Illite/smectite

Illite/smectite (I/S) was identified as a major or minor component in all the separated <2  $\mu$ m fractions with the exception of the sample from Pumpherston 1, 800ft. Peak positions and Newmod II<sup>M</sup>-modelling suggest varied compositions for the I/S in terms of composition (% illite, % smectite), structural ordering expressed as Reichweite numbering (*R*) and crystallite size distribution.

Most commonly, the I/S has an 85% illite, 15% smectite composition, is *R*1-ordered and has a crystallite distribution with a mean defect-free distance of 10 layers (10Å units) and a size range varying from 1 - 30 layers. Ethylene glycol traces show typical broad features at ~12.0, 9.7 and 5.15Å (Figure 6). Such characteristics were identified in 23 of the 50 samples analysed.

Air-dry, glycol and heated peak positions together with Newmod II<sup>M</sup>-modelling suggest that the next most common I/S species has a more evolved 92% illite, 8% smectite composition, is *R*3-ordered and a similar crystallite distribution with a mean defect-free distance of 10 layers (10Å units) and a size range varying from 1 – 30 layers. Ethylene glycol traces clearly resolve a characteristic  $d_{001/004*}$  peak at ~11.1Å, suggesting long-range *R*3-ordering (e.g. Figure 7).



Figure 6. Example <2  $\mu$ m fraction XRD traces for the most common illite/smectite in the sample batch - an illite-rich (~85%), R1-ordered species, sample Pumpherston 1, 2480ft.



Figure 7. Example <2  $\mu$ m fraction XRD traces for the more evolved illite/smectite identified in many of the samples – an illite-rich (92% illite), R3-ordered species, sample Glenrothes 1036.1 ft.

Less evolved I/S species were identified from their XRD characteristics in samples from the Glenrothes, Duloch 3, Duloch 3A and Kelty Bridge 1 boreholes. The I/S in these samples is characterised by a

'superlattice' – a very distinctive, low angle peak typically positioned at ~25Å on the air dry trace which 'swells' to ~26.5Å following ethylene glycol-solvation (Figure 8). Approximately rational sub-order peaks (e.g. ~13.1, 8.9, 5.27 Å) were also observed on the ethylene glycol-solvated trace. Such characteristics suggest that the I/S species is close to a rectorite (*R*1-ordered, 50% illite, 50% smectite) composition. NEWMOD II-modelling suggests *R*1-ordering and variations between 55 and 62% illite for the Midland Valley of Scotland samples. Crystallite size distributions typically show mean defect-free distances of 10 layers (10Å units) and a size range varying up to 25 layers.



Figure 8. Example <2  $\mu$ m fraction XRD traces for a less evolved illite/smectite identified in a few of the samples – a 62% illite, 38% smectite, R1-ordered species, sample Duloch 3, 371.7 ft. Note the distinctive 'superlattice' peak at 26.5 Å on the ethylene glycol-solvated trace.

### 3.2.3 Kaolinite

Kaolinite was also identified by its characteristic air-dry basal spacings of ~7.1 and 3.58Å which remain invariant after glycol-solvation and heating to 375°C but which disappear after heating at 550°C due to the meta-kaolinite's X-ray amorphous state. Kaolinite was identified in all the clay mineral assemblages with the exception of a few samples (Pumpherston 1, 800ft; Glenrothes, 628.1, 635.2, 734.6 ft; Duloch 3A, 530.5 ft).

Kaolinite generally forms a major component (mean 37%) of the clay mineral assemblages of the samples. However kaolinite concentrations are noticeably higher in the samples from the Bargeddie 1, Airth 6, Lawmuir and Milton of Balgonie boreholes together with the upper intervals sampled in the Spilmersford and Kelty Bridge 1 boreholes.

Generally, the kaolinite present in the Midland Valley samples presents moderately sharp XRD peaks suggesting moderate crystallinity. Newmod II<sup>™</sup>-modelling suggests crystallite size distributions with a typical mean defect-free distance of 16 layers (7Å units) and a size range of 1 to 40 layers. Some samples (Pumpherston 1, 2480, 3104.5, 3839 ft; Glenrothes, 1036.1, 1039.9, 1042.3; Duloch 3, 371.7 ft; Kelty Bridge 1, all samples; Spilmersford, 509 ft; Leven Seat 1, 4810 ft) exhibit sharper kaolinite XRD peaks, reflecting a greater degree of crystallinity and Newmod II<sup>™</sup>-modelling suggests crystallite size

distributions with a mean defect-free distance of 25 layers (7Å units) and a size range of 1 to 55 layers for these samples. The two shallowest samples from the Lawmuir 1A borehole (150.7 and 231.3 ft) and the deepest sample from the Bargeddie 1 borehole (3176.75 ft) show relatively broad kaolinite XRD peaks suggesting a more poorly crystalline species is present. Newmod II<sup>™</sup>-modelling suggests crystallite size distributions with a typical mean defect-free distance of 10 layers (7Å units) and a size range of 1 to 30 layers for these three samples.



Figure 9. Example <2 μm fraction XRD traces to illustrate a poorly-crystalline, kaolinite-rich clay mineral assemblage, sample Lawmuir 1A, 150.7 ft.

### 3.2.4 Chlorite

Chlorite was identified by its characteristic air-dry, glycol-solvated basal and heated 375°C spacing peaks at 14.2, 7.1, 4.72 and 3.54Å and particularly the presence of a peak at ~13.9Å after heating for 2 hours at 550°C.

Chlorite forms a minor component (mean 7%) of many of the clay mineral assemblages but is absent from all the samples taken from the Bargeddie 1, Spilmersford and Lawmuir 1A boreholes, the shallowest samples from the Kelty Bridge 1 borehole and all but the deepest sample in the Milton of Balgonie 3 borehole. Significantly higher proportions of chlorite were identified in the clay mineral assemblages of samples from the Salsburgh 2, Glenrothes (shallower) and Duloch 3 boreholes.

Peak intensity ratios and Newmod II<sup>™</sup>-modelling suggests that the chlorite species identified in most of the samples are of intermediate Fe/Mg compositions. However the chlorite in most of the samples from the Glenrothes borehole (635.2, 734.6, 1036.1, 1039.9 and 1042.3 ft) and the sample from the Duloch 3A borehole (530.5 ft) appears to be Mg-rich.

Newmod II<sup>™</sup>-modelling suggests crystallite size distributions with a typical mean defect-free distance of 10 layers (14Å units) and a size range of 1 to 33 layers.

The chlorite identified in three of the samples (Pumpherston 1, 800ft; Glenrothes, 628.1 ft and Duloch 3, 371.7 ft) showed different characteristics to that in the other Midland Valley samples. In these samples,

the chlorite even-order basal peaks ( $d_{002}$  and  $d_{004}$ ) are very intense and have reduced peak widths when compared to the chlorite odd-order basal peaks ( $d_{001}$ ,  $d_{003}$  and  $d_{005}$ ). Newmod II<sup>M</sup>-modelling explains such characteristics by the presence of a small number (~10%) of serpentine interlayers in an otherwise *R*0-ordered, Fe-rich chlorite structure.

### 3.2.5 Talc

Small quantities of talc were identified in four of the Midland Valley samples (Glenrothes, 628.1 and 635.2 ft; Kelty Bridge 1, 960 and 1380 ft), principally by its characteristic air-dry, glycol-solvated basal and heated 375/550°C spacing peak at 9.3Å.

### 3.2.6 Non-clay minerals

XRD analysis also indicates the presence of variable amounts of non-clay minerals in the <2  $\mu$ m fractions. These include quartz, plagioclase feldspar, siderite, calcite and pyrite. Particularly greater amounts of quartz were identified in the <2  $\mu$ m fraction isolated from the sample from the Salsburgh 2 borehole, 3463.33 ft. Despite applying repeated buffered-leaches, calcite and siderite were found to form a trace component of a few of the <2  $\mu$ m fractions obtained from the carbonate-rich samples (Tables 4 and 5).

# 4 Discussion

The submitted samples from the Bargeddie 1, Salsburgh 2, Stewart 1, Airth 6, Craighead 1, Cousland 6, Milton of Balgonie 3, Pumpherston 1, Glenrothes, Duloch 3, Duloch 3A, Kelty Bridge 1, Spilmersford, Leven Seat 1 and Lawmuir 1A boreholes present a range of mineralogical assemblages including quartz-rich, carbonate-rich and phyllosilicate/clay mineral-rich lithologies.

### 4.1 Comparison with previous analyses

Peer-reviewed published mineralogical analyses of fine-grained sedimentary rocks from the Lower Carboniferous strata of the Midland Valley of Scotland are limited to the studies of Wilson *et al.* (1972) and Monaghan *et al.* (2012).

Using an XRD, electron microscopy and differential thermal analysis approach Wilson *et al.* (1972) studied the clay mineralogy of 129 varied-lithology samples from the complete Carboniferous succession, mostly from outcrop with only a few borehole samples representing the Passage Formation. The clay mineralogy of the Carboniferous samples was found to be composed of kaolinite and illite but peak symmetry changes following glycerol-treatment suggested the minor presence of interstratified expansible layers. The illite was found to be dioctahedral as shown by the (060) reflection at 1.50 Å and the abundant kaolinite tended to be moderately well-ordered. The more detailed mineralogical analysis presented in the present study would appear to be entirely consistent with these early results.

Modal mineralogical analysis carried out by image analysis of energy-dispersive x–ray microanalysis (EDXA) coupled with backscattered scanning electron microscopy (BSEM) showed that mudstones and siltstones from the Ballagan, Upper Limestone and Lower Coal Measures formations were commonly composed of illitic clay with minor quartz, muscovite, biotite and chlorite (Monaghan *et al.* 2012).

Commercial whole-rock and clay mineral XRD analyses (Composite Energy 2010a, available from the BGS National Geological Records Centre) were produced for three Midland Valley boreholes – Leven Seat 1 (9 samples, 580 – 1900 ft), Bargeddie 1 (10 samples, 2360 – 3166 ft) and Inch of Ferryton (4 composite samples, 5000 – 5750 ft). Samples from Leven Seat 1 and Bargeddie 1 boreholes were also included in the present study, although these were taken from greater depths than the commercial analyses.

Further whole-rock XRD analyses for four samples from the Black Metals Marine Band (Composite Energy 2010b) were also produced from three further boreholes - Airth 6 (1 sample, 3016 ft), Bandeath 1 (1831 ft) and Longannet 1 (2 samples, 3427 and 3432 ft).

In general terms the commercial analyses (Composite Energy 2010a, b) identify a similar range of minerals to those in the present study but their concentrations appear to be slightly different. Assuming that the previous studies have similar levels of accuracy to the present study (±2.5%), this is perhaps unsurprising as the samples analysed in each study represent different depth intervals and positions within the basin. That is, well logs for two of the three wells sampled by Composite Energy indicate a more siliciclastic-rich, shale-poor succession or a thinner sequence than average, being located towards the basin margin (Leven Seat 1) or a local high (Inch of Ferryton 1). The triplot shown in Figure 10 compares the previous commercial analyses with the present study. The Composite Energy (2010a) data produces an average composition of ~45% phyllosilicate/clay minerals, ~11% carbonate and 44% QFP indicating an approximately similar average carbonate content but a QFP-rich and phyllosilicate/clay mineral-poor composition compared to the present study.

Triplot comparison of whole-rock mineralogies discriminated on the basis of borehole location (where samples have been analysed in both studies) and stratigraphy are shown in Figures 11 and 12. Both plots show mineralogical differences, particularly noticeable in carbonate content, which would seem to be attributable to the different depth intervals and well positions represented.

Commercial clay mineral analyses of <2  $\mu$ m fractions (Composite Energy 2010a) indicate similar illite, kaolinite, I/S and chlorite assemblages to those identified in the present study. The Composite Energy (2010a) study consistently identified the illite-smectite as an *R*1-ordered species with composition 70-80% illite and the kaolinite was predominantly described as moderately well-crystallised. These findings

are very similar to those from the present study, although the I/S composition is more variable and generally more illitic in the present study.

While the majority of the findings of the present study are broadly in-line with previous studies, the identification of talc in samples from both the Glenrothes and Kelty Bridge 1 boreholes has not been previously recorded. Similarly the siderite-rich nature of the ironstone (with black carbonaceous mudstone) from the Bargeddie 1 borehole (3170 ft) has not been previously noted.

The extremely clay-rich nature of the samples from the Lawmuir 1A borehole is also interesting. Their clay-rich nature together with their often kaolinite-dominated clay mineralogy suggests that the Lawmuir Formation samples may represent either seat earths, formed as a result of emergence of the sediment and colonisation by land plants or possibly tonstein horizons, formed by the *in situ* alteration of volcanic ash. Either of these possibilities is consistent with the character of the Lawmuir Formation and its position overlying the Clyde Plateau Volcanic Formation. Geochemical and petrographic analysis would be necessary to prove which of these origins is correct.

Both the present and previous mineralogical studies of the Midland Valley of Scotland samples indicate that these shales have significantly different mineralogy to the USA unconventional gas shales most suited to fracture simulation (<35% clay content (Jarvie 2012a) or <50% (Bowker 2007)). Compared to triplots of USA productive shales (Hart *et al.* 2013, Gamero-Diaz *et al.* 2013), a significant proportion of the Midland Valley of Scotland samples are more phyllosilicate/clay mineral-rich and carbonate-poor. Such mineralogical differences are likely to produce different engineering behaviours for the Midland Valley of Scotland shales compared to the USA shales (see section 4.3). Samples with TOC values >2% do not appear to be related to clay or QFP contents, though it is noticeable that the high carbonate content samples have TOC values <2% (Figure 10).



*Figure 10. Triplot to illustrate the whole-rock mineralogy of the Midland Valley of Scotland samples compared to previous commercial analyses, differentiated on the basis of TOC content.* 

APPENDIX E TO THE CARBONIFEROUS SHALES OF THE MIDLAND VALLEY OF SCOTLAND: GEOLOGY AND RESOURCE ESTIMATION



*Figure 11. Triplot to illustrate the whole-rock mineralogy of the Midland Valley of Scotland samples compared to previous commercial analyses, discriminated on a borehole basis* 



*Figure 12. Triplot to illustrate the whole-rock mineralogy of the Midland Valley of Scotland samples compared to previous commercial analyses, discriminated on a stratigraphic basis* 

## 4.2 Maturity and burial history

The relatively small number of samples submitted from each borehole precludes a detailed commentary on downhole variation but the extracted clay mineralogies provide an indication of the maturity and burial history of the samples, relevant to their potential as unconventional gas or oil sources and their engineering behaviour.

Because of their small grain-size and thermodynamic metastability, clay minerals are particularly sensitive to changes in the shallow crustal conditions that control the thermal history of sedimentary basins. Following from the seminal work of Hower et al. (1976), clay mineral transformations (reactions) resulting from burial in sedimentary basins have been widely studied and increasingly used to model basin thermal history. During sedimentary burial, a progressive series of clay mineral reactions converts soft mud to hard lithified mudstone and shale. Quantitatively, the most important series of reactions responsible for the lithification of mud is the progressive transformation of smectite to illite via a series of intermediate illite/smectite (I/S) mixed-layer minerals. Progress of this series of dehydration reactions increases the density of the mudstone by mobilising fluids, and also reducing pore-space as a new, bedding-parallel illite invades and fills voids (Merriman & Peacor 1999). The progress of the smectiteto-illite reaction can be measured using X-ray diffraction (XRD)-based techniques such as computer modelling of the percentage illite in I/S, and measuring changes in 'illite crystallinity' using the Kübler index (KI). Changes in KI caused by diagenetic burial and very low-grade metamorphism have been correlated with transmission electron microscopy (TEM) measurements of illite crystallite thickness from a variety of mudrocks including mudstone, shale and slate samples (e.g. Warr & Nieto 1998, Merriman & Peacor 1999, fig. 2.19). These show that during burial diagenesis, illite crystallites progressively increase in mean thickness from 2 or 3 (10-Å) layers to 20-25 (10-Å) layers, prior to the onset of very low-grade metamorphism. Progressive increases in illite crystallite thickness are not reversed by basin inversion and uplift and can be used to estimate maximum burial depth, particularly when used with other indicators of thermal maturity such as vitrinite reflectance or apatite fission track analysis.

Reaction-progress in clay minerals in relation to changes observed in organic materials have been used to construct a Basin Maturity Chart summarizing these depth-dependent changes (Merriman & Kemp 1996).

The clay mineral data for the Midland Valley of Scotland borehole samples are plotted on the Basin Maturity Chart in Figure 13, assuming a geothermal gradient of 25°C/km (in accordance with Vincent *et al.*, 2010), to aid interpretation of their burial history.

The majority of the samples analysed contain an *R*1-ordered I/S, ~85% illite (West Lothian Oil-Shale Formation in Bargeddie 1, Salsburgh 2, Stewart 1, shallow Kelty Bridge 1, Craighead 1 and Cousland 6; Gullane Formation in shallow Stewart 1, Spilmersford, Pumpherston 1; Pathhead Formation in deep Milton of Balgonie 3, Lower Limestone Formation in Kelty Bridge 1 and Lawmuir Formation in shallow Lawmuir 1A), which places these samples in the Deep Diagenetic metapelitic zone and suggests maximum burial temperatures of ~150°C, equivalent to burial of perhaps ~6 km at an average geothermal gradient of ~25°C/km. In terms of hydrocarbon zones, the clay data suggest that these samples generally fall within the Light Oil/Wet Gas maturity zones (Figure 6).

The more evolved R3-ordered I/S (~92% illite) present in some of the Midland Valley samples (Gullane Formation in deep Stewart 1, Black Metals Marine Band in Airth 6, Lower Limestone and Pathhead formations in Milton of Balgonie 3, Ballagan Formation in Glenrothes, Spilmersford, Inverclyde Group in Leven Seat 1 and Lawmuir Formation in deep Lawmuir 1A) suggests burial temperatures of ~200°C and places these samples at the transition from the Deep Diagenetic metapelitic zone to the Low Anchizone, equivalent to burial of perhaps ~8 km at an average geothermal gradient of ~25°C/km. In terms of hydrocarbon zones, the clay data places these samples at the Wet Gas/Dry Gas transition zone (Figure 13).

The less mature *R*1-ordered, ~55% illite I/S identified in the Pathhead Formaiton (Glenrothes) and West Lothian Oil-Shale Formation (Duloch 3, 3A and deep Kelty Bridge 1) samples would seem to suggest shallower maximum burial of perhaps 4 km. These samples would appear to have only reached the Shallow Diagenetic metapelitic zone and perhaps a maximum burial temperature of 100°C. In terms of

hydrocarbon zones, the clay data suggest that these samples fall within the Heavy Oil zone or are perhaps even Immature (Figure 13).

While the identification of less mature I/S in all the samples from Duloch 3 and 3A may indeed suggest shallower burial of the Lower Carboniferous strata, the burial history of these rocks in the Glenrothes and Kelty Bridge 1 boreholes appears to be more complicated.

In the Glenrothes borehole, the identification of the ~55%, R1-ordered I/S in the samples from the Pathhead Formation (628.1 and 635.2 ft) is followed by the identification of ~90%, R1- (734.6 ft) or 92%, R3-ordered I/S in the Ballagan Formation (1036.1 to 1042.3 ft). Such an increase in the illitization of the I/S over such a small depth interval could be interpreted as suggesting the removal of significant amounts of intervening strata. Indeed, there is a large unconformity and thin sequence between these two formations in the borehole (see Appendix C, Figure C6). However, perhaps more likely is that the shallower, Pathhead Formation samples contain a greater volcanogenic input or have undergone diagenetic or hydrothermal retrogression compared to the deeper samples. Bentonites, rocks predominantly composed of altered volcanogenic material, are known to illitize less quickly than mudstones reflecting the metastability of their clay minerals (e.g. Li et al. 1997, Masuda et al. 2001). Examples of retrograde diagenesis have been noted on both a regional (e.g. Nieto et al. 1994) and a more localised scale (e.g. Jiang et al. 1990). The more localised alteration was associated with fluid activity close to a major fault zone. Similarly, hydrothermal reactions may retrogress clay mineral authigenesis (e.g. Kemp et al. 2005, Henry et al. 2007). The Glenrothes borehole is sited only a few kilometres from the East Ochil Fault, a major basin-bounding fault, which may have provided a fluid conduit during intrusion of the Midland Valley Sill-complex. Such a hypothesis would appear to be reinforced by the unusual occurrence of talc in the shallow Glenrothes samples.

In the Kelty Bridge 1 borehole, an 85%, *R*1-ordered I/S was identified in the shallowest samples from 110 and 540 ft but the deeper samples contain a less mature ~55%, *R*1-ordered I/S (960 and 1380 ft). Such identifications infer a volcanogenic input or hydrothermal retrogression. Organic vitrinite reflectance (VR, R<sub>0</sub>%) data provide further evidence for igneous intrusion and hydrothermal alteration just below the borehole total depth (main report Figure 58). Again the unusual identification of talc in the deeper samples would appear to provide further evidence for such a suggestion.

In overall terms, the suggested clay mineral maturities appear to be in close agreement with maturities obtained from VR data (main report, section 3.6). Most of the succession is mature but some parts, particularly the deeper parts of the succession, have been affected by igneous intrusion resulting retrogressed clay minerals but  $R_0$ % values >2. It is widely recognised that clay mineral maturation is relatively slow compared to organic materials (e.g. Merriman 2005). The close agreement between the clay mineral and organic matter maturities would therefore seem to suggest that sedimentary burial in the Midland Valley of Scotland has been relatively slow, under approximately 'normal' geothermal gradients.

## 4.3 Inferred engineering properties

The words "ductile" and "brittle" have emerged as two key descriptors for characterising unconventional gas or oil shales in relation to hydraulic fracturing. The former are usually relatively organic (TOC)- and clay-mineral rich, while the latter are considered to be more enriched in "silica" (i.e. biogenic and/or detrital quartz)- and/or carbonate (calcite/dolomite) minerals (Slatt 2011). Mineralogical data from the Barnett Shale and many other productive shales in the USA suggest that explorationists should target shales with low proportions of clay minerals (generally less than 50%) to allow successful fracture stimulation (Bowker 2007). Indeed, mineralogy appears to be the key factor for characterising the best Barnett Shale wells with greatest production from zones with 45% quartz and only 27% clay (Bowker 2003).

Common measures of rock strength and deformation are Young's modulus and Poisson's ration; these properties and others used characterise a rock as brittle or ductile have not been measured in this study. However, engineering properties can be simplistically related to mineralogy, with caveats relating to rock anisotropy and the form of quartz (biogenic, detrital etc) in the rock.

In order to characterise shale mineralogy in terms of engineering behaviour a simplistic 'Brittleness Index' (*BI*, Slatt 2011) may be calculated using the formula:

#### BI = (%Silicates + %Carbonates)/(%Silicates + %Carbonates + %Clays + %TOC)

High values (e.g. 0.7) are considered to indicate brittle shales, whereas low values (e.g. 0.3) may indicate ductile behaviour. *BI* values for the Midland Valley of Scotland samples from this study and previous studies are summarised in Table 6. It is important to note the 'Brittleness Index' is a simplistic indicator of rock geomechanical properties, that are influenced by depositional and diagenetic processes, rock fabric etc (Hart *et al.* 2013). As such, further detailed work on the geomechanical properties, diagenesis and fabric of the Midland Valley of Scotland shales is recommended.

Individual sample *BI* values for the present study are variable and range from 0.00 to 0.82 with a mean value of 0.39. The previous commercial analyses (Composite Energy 2010a) summarised in Table 6 for the West Lothian Oil-Shale, Pathhead and Lower Limestone formations present *BI* values that indicate slightly more brittle behaviour on average than the BGS samples. As discussed above, this is likely because two of the three wells sampled by Composite Energy (Leven Seat 1 and Inch of Ferryton 1) are more siliciclastic rich than average, being located towards the basin margin or a local high.

Ctuationaukia unit	This st	udy	Previous studies			
Stratigraphic unit	No. samples	Mean BI	No. samples	Mean BI		
Black Metals Marine Band, Limestone Coal Fm	3	0.31	4	0.24		
Lower Limestone Fm	3	0.46	9	0.54		
West Lothian Oil-Shale Fm	17	0.45	13	0.51		
Pathhead Fm	4	0.31	1	0.57		
Lawmuir Fm	4	0.19				
Gullane Fm	11	0.34				
Ballagan Fm	7	0.40				
Inverclyde Group	1	0.82				

Table 6. Summary Brittleness Index data for the Midland Valley of Scotland samples

Importantly, the clay mineral maturity of the Midland Valley of Scotland borehole samples may also be related to the microfabric, lithology and ultimately therefore to the engineering properties of the sampled lithologies. However, it should be noted that these relationships may have been complicated by the possible presence of volcanogenic material and/or hydrothermal retrogression.

As detailed by Merriman & Peacor (1999), the Deep Diagenetic Zone is characterised by claystone, mudstone and shale pelitic lithologies. Claystones and mudstones lack the fissility of shales that split easily into thin sheets along planes approximately parallel to bedding. At outcrop, claystones and mudstones commonly spall into centimetre-size blocks along polygonal shrinkage cracks, reflecting the presence of illite/smectite. Microfabrics show an overall bedding-parallel orientation. Therefore, on the basis of clay mineral maturity, the majority of the samples analysed in this study would be expected to show such characteristics.

	one (	(C)		Ν	ludrocks			Sandstones		Rr%	5	0 al David		
BASIN MATURITY	Metapelitic Z (depth, km	Temperature	di-smectite - muscovite 2:1	Kubler Index IC (∆°20)	tri-smectite - muscovite 2:1	kaolinite - pyrophyllite 1:1	di-smectite - muscovite 2:1	tri-smectite - chlorite di/tri - chlorite 2:1	kaolinite - pyrophyllite Fe-serpentine 1:1	w Vitrinite Reflectance F	Hydrocarbo Zones	Coal Rank and Volatile Matter (%)	Conodont Alteration Index(CAI	
IMMATURE	Shallow Diagenetic		di-smectite		tri-smectite	a olinite	di-smectite	saponite	— berchierine (adinite) ——— —————————————————————————————————		Immature Heavy	Peat Lignite Sub. Bituminous	1 .yellow	PDB (Glenrothes) WLO (Duloch 3, 3A, deep Kelty Bridec J
MATURE	ep Diagenetic		Illite	~0.60	porrensite		illite/smectite		- berthierine/chlorite	0.75	Oil Light Wet Gas	45 40 35 30 25 20	2 light brown 3	WLO (Bargeddie 1, Salsburgh 2, Stewart 1, shallow Kelty Bridge 1, Craighead 1, Cousland 6) GUL (shallow Stewart 1, Spilmersford, Pumpherston 1) PDB (deep Milton of Balgonie 3) LLGS (Kelty Bridge 1) LWM (shallow Lawmuir 1A)
SUPER - MATURE	Anchizone	~200	90% illite	0.42	corrensite/chlorite	kite (nacrite)		corrensite (chlorite	dokte	2.00	Dry Gas	Bituminous 15 Semi- Anthracite	4 dark brown	GUL (deep Stewart 1) BKME (Airth 6) LLGS (Milton of Balgonie 3) PDB (shallow Milton of Balgonie 3 BGN (Glenrothes, Spilmersford) INV (Leveseat 1) LWM (deep Lawmuir 1A)
	Low		te (phengite) —	~0.3		đi	te (phengite) —		tit.	3.00		Anthracite		
SUPER - MATURE	High Anchizone	~300	muscovi	0.25	chlorite	pyrophylite	muscovi	- chlorite	indonya	4.00	Over- mature		5 black	
	Epizone	-300		0.25						4.00		Meta- Anthracite	5.5	

Figure 13. Clay mineral maturity data for the Midland Valley borehole samples plotted on the Basin Maturity Chart (Merriman & Kemp 1996). Note that burial depths are for a 'normal' geothermal gradient of 25°C/km. Stratigraphic codes are explained in Table 1.

# **5** Conclusions

This report summarises the results of whole-rock and <2  $\mu$ m clay mineral X-ray diffraction analyses carried out on a suite of 50 samples of Carboniferous fine-grained sedimentary rock samples collected from boreholes located in the Midland Valley of Scotland.

Several points were noted as a result of these analyses:

- The samples are composed of variable proportions of quartz, feldspar (plagioclase and K-feldspar), carbonates (calcite, dolomite, ankerite/Fe-dolomite and siderite), clay minerals/phyllosilicates ('mica', kaolinite, chlorite), pyrite and jarosite.
- An average composition for the samples would be ~59% phyllosilicates/clay minerals, ~9% carbonate minerals and ~32% QFP (quartz, feldspar, pyrite). Such compositions are considerably more clay mineral-rich and carbonate-poor than USA unconventional gas-producing shales.
- <2 μm clay mineral assemblages are generally composed of various amounts of illite, illite/smectite (I/S), kaolinite and an intermediate Fe/Mg chlorite. Minor proportions of talc were also identified in a few samples. Various I/S compositions were identified. Most samples contain an R1-ordered I/S (~85% illite) with a more evolved R3-ordered I/S (~92% illite) identified in many of the deeper samples. A less mature R1-ordered, ~55% illite I/S was identified in a few samples.
- Moderately crystalline kaolinite typically forms a major component and intermediate Fe/Mg chlorite a minor component of the clay mineral assemblages. Kaolinite and chlorite can form a more significant component and become more Mg-rich in some boreholes. An interlayered chlorite/serpentine was identified in a few samples.
- The results from this study are broadly in-line with previous peer-reviewed published and commercial analyses.
- The sample's clay mineral assemblages provide an indication of the maturity and burial history of the samples, relevant to their potential as unconventional gas sources and their likely engineering behaviour.
- Clay minerals suggest that the majority of the samples have been buried to ~6 km at 'normal' geothermal gradients (~25°C/km) and probably represent the Light Oil/Wet gas maturity zones. These samples are likely to show a bedding parallel microfabric.
- The R3-ordered I/S (~92% illite) present in fewer of the samples places these in the Wet Gas/Dry Gas transition zone, equivalent to burial of perhaps 8 km at normal geothermal gradients. Such burial typically produces a bedding-parallel microfabric.
- The presence of an *R*1 55% illite I/S in a few samples would place these samples in the Heavy Oil or even Immature zone, equivalent to burial of perhaps ~4 km at normal geothermal gradients. However, other evidence suggests that the presence of this I/S is more likely to represent either a greater, initial volcanogenic component to the shale or that these rocks have undergone diagenetic or hydrothermal retrogression.

#### References

See main report

# Appendix F Estimation of total organic carbon in the Carboniferous shales of the Midland Valley of Scotland by log analysis

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# **1.Summary**

This report documents the calculation of total organic carbon (weight percent (TOC wt%)) from geophysical logs across the Carboniferous units of interest for prospective shale oil and shale gas in the Midland Valley of Scotland. Geophysical data were available from wells drilled in the 1980s stored in the British Geological Survey database. These were extracted, verified and analysed using the Passey sonic method to give vertically continuous wt% TOC curves for each well. Estimated clay volume curves were also calculated to apply discriminators to the tabulated outputs. Intervals with clay volume values greater than 0.5 (50%) were considered "net" for the average wt% TOC and net to gross (N/G) calculations, and intervals with greater than 2 wt% TOC were considered organic-rich "pay" in the pay to gross (P/G) values calculated for each of the Carboniferous clay units listed:

- Limestone Coal Formation
- Lower Limestone Formation
- West Lothian Oil-Shale Formation
- Gullane Formation



Figure 1 Wells selected for the study across the Midland Valley of Scotland. Wells with core sample TOC data are shown in blue.

From the small limited sample of well data examined, the formations with the highest calculated wt% TOC were the Limestone Coal Formation and Lower Limestone Formation. These had average wt% TOC greater than 4% in organic-rich shales. The West Lothian Oil-Shale Formation was the thickest formation, over 100 m thick in wells which detected it. It showed great variability in calculated TOC and at certain intervals discrete TOC rich shales were identified. The Gullane Formation was similar to the West Lothian Oil-Shale Formation, with high shale content and discrete intervals of high calculated TOC, although it is restricted to eastern wells.

Geographically the wells can be split into eastern and western wells. The western wells (*Craighead 1* and *Bargeddie 1*) showed more organic-rich shales with higher calculated wt% TOC and pay to gross (P/G). Eastern wells had lower quality data and after calculations showed leaner shales giving lower calculated wt% TOC and P/G, these wells however showed discrete intervals of higher calculated TOC.

Depths and thicknesses in this Appendix are given in metres.

# **2.Introduction**

Assessing Total Organic Carbon (TOC) values of shales for use in shale gas and shale oil resource estimates was traditionally done using core samples or less reliable cuttings samples. Core data are very limited both geographically and stratigraphically, and cuttings are affected by a number of drilling-related problems. Recently, however, assessment of weight percent (wt%) TOC has been undertaken using analysis of geophysical well logs. This has enabled many wells with no core data to be analysed to give calculated TOC wt% values and a complete vertical assessment of TOC wt% per well. Applied across the basin in question, this will improve resource estimates and can be a valuable aid to identifying likely productive intervals.

During the 1980s numerous boreholes were drilled and logged to assess hydrocarbon prospectivity in the Midland Valley of Scotland. Some of the geophysical well log data were stored and/or digitised by the British Geological Survey.

The key aim for this well log study is to calculate TOC estimates in the Midland Valley of Scotland and produce graphical logs showing this for 5 wells. The intervals of interest are all in the Carboniferous and include the Limestone Coal, Lower Limestone, West Lothian Oil-Shale and the Gullane formations (see main report Table 4).

# **3.Method**

The method used for the study is outlined below:

- 1. Literature Research: Research of literature relating to methods of deriving TOC weight percent from geophysical logs and Level Of Maturity (LOM) from vitrinite reflectance. Furthermore, research of good protocol using Interactive Petrophysics (IP) and RECALL (the British Geological Survey log database).
- 2. Locating and Uploading Data: Relevant geophysical log curves from RECALL were extracted and if necessary multiple curves combined to produce a single log curve per well. Total Organic Carbon (TOC) values were located for specific wells with core data available and uploaded. All data were loaded into IP for further analysis.

- 3. Verification of Data: Verification of formation tops and log quality was undertaken using a variety of sources, and if inconsistencies were found the most reliable source of data was used.
- 4. Analysis and Calculations using Geophysical Well Logs: Various calculations were undertaken to determine Level of Maturity (LOM, for certain formations) for use in IP, TOC (from the Passey method) and the Volume of Clay (VCI).
- **5. Presentation of Results:** The TOC was displayed with graphical logs, histograms and tabulated plots per formation. Statistics for TOC were computed for each formation, including averages, max/min and thicknesses of high TOC intervals relative to total reservoir thickness.

## 3.1 Literature search

Passey et al. (1990) developed a method to quantatively calculate TOC in weight percent from level of maturity (LOM) estimations and log responses in lean versus organic rich shales using a log overlay method known as DlogR. The resistivity curves were overlaid against either sonic, density or neutron logs at particular scales and shaded where they overlaid to indicate organic richness. Their method was chosen for this study as it appears to be an industry-accepted method for calculation of TOC for shale gas and test results and compares favourably with those derived by other calculation methods (not described here).

Hood, Gutjahr and Heacock (1975) developed the LOM scale needed in the Passey equation. The scale describes a single numerical scale applicable to the thermal range of interest. It is based on a combination of coal rank, vitrinite reflectance and spore carbonization. They inferred that Vitrinite Reflectance (known as VR or  $R_o$ , the latter will be used in this report) is directly related to LOM; therefore with accurate  $R_o$  values, LOM can be calculated.

A literature review for Raymond (1991) can be found in the main report

## 3.2 Locating and uploading data

The well list provided contained 8 wells which were all contained in the BGS log software RECALL.

- a. The first step was to extract the well data from RECALL as \*.las files which can be imported into IP. Many of the wells had digital composite files created, which consist of a suite of logging curves, giving a complete log from top to bottom by combining several sections of the well into a continuous data set.
- b. The TOC and  $R_o$  data for the wells with available core data were extracted from a provided database. The TOC were then uploaded into IP. Use of the  $R_o$  data is described in step 5.
- c. All wells in the Midland Valley of Scotland were considered, but few had the necessary geophysical logs. Even for wells with the necessary logs, some had issues (e.g. incorrect scaling or faulty logging; Leven Seat 1, Milton of Balgonie 1, Firth of Forth 1) which resulted in their omission from the study.

## 3.3 Verification of data and quality checking

The data extracted required verification as follows:

- a. The uploaded digital curves in IP were compared to those on the composite log plot scans:
  - To verify the curve responses with depth and their scales. Any differences between the digital plot and log plot composite were noted.

- Any data gaps in the digital curves (often as a result of no data recorded, for example across casing shoes or due to logging problems) were filled by a straight line and recorded.
- b. The formation tops provided (Appendix C) were loaded into IP and also compared with the composite log plots (if disagreements between the two depths arose, the formation tops provided were chosen preferentially).
- c. The logging curves were assessed for quality by checking for unusual responses, checking responses were within tolerance (where suitable curves were available) and noting where poor hole conditions affected the data:
  - CALI, the caliper curve, measures hole size. This showed wash outs (enlargement) in some places, particularly over the clay intervals, which can detrimentally affect other curve responses (in particular those which require pressing against the borehole wall to read correctly, such as the density or neutron data). Where the caliper is open to its maximum extent (curve flatlining), data from those tools that rely on borehole wall contact were treated as suspect or unreliable.
  - DRHO the density correction curve should fall within the -0.1 and 0.1 range for good density (RHOB) data. Outside of this range, the density data were treated as suspect or unreliable.

Many of the wells had intervals of poor density data (DRHO out of tolerance), reinforcing the use of sonic data (less affected by poor hole conditions) for the Passey TOC calculations for these wells.

## 3.4 Analysis and Calculation of Geophysical Well Logs

The main objective of this study was to produce logs showing the TOC of wells across the basin; these are accompanied by statistical outputs for each well. To be able to calculate the TOC, the LOM values were established. Also, to discriminate shale source from sand/limestone reservoir a volume of clay cut-off was required.

*Volume of Clay (VCl):* The volume of clay parameter is calculated based on the gamma ray response. In general a higher GR value is indicative of a larger percentage of clay. The output curve is scaled between 0-1 (1 being 100% clay and 0 being 100% 'clean'). It was used as a discriminator in subsequent calculations, to remove intervals with less than 50% clay (i.e. those considered unlikely to be prospective for shale gas and oil). Each well was subdivided into three intervals (Limestone Coal /Lower Limestone formations, West Lothian Oil-Shale Formation and Gullane Formation) and processed individually to define the GR minimum and maximum parameters required. Neutron-density data, where good quality was available, was used to cross-verify the GR-derived VCl curves.

*Level Of Maturity (LOM)*: A key parameter in the Passey equation for calculating TOC is the Level of Maturity (LOM). This can be calculated from R<sub>o</sub> values, measured on core samples (Hood et al. 1975). R<sub>o</sub> data were available for three of the five wells studied, for the two wells where  $R_o$  data unavailable were their proximity to other wells

	LOM used (Min-Max, Average)							
Name	L Coal/Lr Lmst	WLO	Gullane					
Bargeddie 1	9.5-11 (10.25)	10.5-11.5 (11)	-					
Carrington 1	8.2-9.8 (9.2)	8.6-10.1 (9.6)	9.9-11.85 (11.2)					
Craighead 1	9.5-11 (10.25)	10.5-11.5 (11)	-					
Kelty Bridge 1	-	9.6-11.2 (10.3)	-					
Straiton 1	-	-	9.2-11.4 (10.6)					

**Table 1**: The range of Level Of Maturity for the study area for each formation.(Average bracketed). WLO=West Lothian Oil-Shale Formation

allowed for similar R<sub>o</sub> values to be used. For *Kelty Bridge 1*, the R<sub>o</sub> values were very high towards the

base due to igneous intrusion influence; therefore a background  $R_o$  was used as suggested by Raymond (1991). As the  $R_o$  generally increases with depth, over the thickness of a formation a range of  $R_o$ 's form, this is represented by a range of LOM values assigned, to incorporate the maximum and minimum potential LOM values for each formation.

*Passey Method for Calculating TOC:* The TOC was calculated using the Passey-method inbuilt IP TOC calculator. Wells with core data were implemented first, to assist in selecting the parameters and calibrating the output TOC curve to the core data where appropriate. The wells were split vertically into 3 zones, representing the Limestone Coal/Lower Limestone formations, West Lothian Oil-Shale Formation and Gullane Formation, and the overlay adjusted in each zone to match core data. The density and neutron overlay plots were used to verify those of the sonic.

The output TOC curves were calculated first at the average LOM (Table 1 (bracketed values)), to give a TOC\_M curve (the "most likely" value). The LOM parameters were then adjusted to the maximum and minimum values in Table 1 and the TOCs recalculated (TOC\_L and TOC\_H, respectively), to represent the sensitivity of TOC outputs to the LOM parameter. This is displayed as the blue shading on the TOC curve in the graphical log plots, (Higher LOM values give **lower** TOC values for a given set of logs).

## 3.5 **Presentation and Explanation of Results**

The main findings and geographical trends are documented in the section 4 by formation summary, and tables and maps are also included.

Results by well are included in the Appendix in the form of graphical log plots and tables of summary statistics. The tables contain TOC statistics, Net/Gross and Pay/Gross values from the formations of interest with cut-offs applied to discriminate clean intervals, reservoirs and poor TOC values as listed below:

- TOC statistics: Minimum, maximum and mean values are included.
- Net/Gross: Indicates the amount of each formation that is considered to be shale. Intervals where Volume of Clay (VCI) is greater than 0.5 (50% clay) are included as "Net". Gross is the total formation thickness.
- Pay/Gross values: Indicates the amount of each formation that is considered to be potentially prospective for shale gas and oil. Net intervals where TOC is greater than 2 wt% are included as organic-rich "Pay". Gross is the total formation thickness.
- Pay/Gross for >15 m (50 ft) shale intervals: Indicates the amount of each formation that is considered potentially prospective for shale gas or oil in intervals greater than 15 m. Net intervals where TOC >2 wt% and thickness is >15 m are included as organic-rich "Pay". Gross is the total formation thickness (minor smoothing on the VCl curve removing minor (<1 m) clean intervals was undertaken).</li>

Results were displayed graphically for each well in a six-track log plot. These include in track order (from left to right):

- 1. Formation intervals. Intervals of interest are coloured.
- 2. Measured Depth (MD) below Kelly Bushing (KB) in feet
- 3. Gamma Ray (GR) and Caliper: GR shows natural formation gamma ray response, which tends to be higher in shales. Caliper indicates hole size and can give an indication of enlarged or rugose hole which may affect data quality.
- 4. Volume of Clay (VCl) with the 50% clay cut-off represented by 'clean' and 'shaley' shading.

- 5. The Passey Sonic-Resistivity curves, with yellow shading representing TOC-rich intervals.
- 6. Final TOC values, blue shading to indicate TOC range (between TOC\_L and TOC\_H) and, where possible, Core TOC values.

## 3.6 Assumptions and Limitations

The following assumptions and limitations should be considered when analysing the results and graphical TOC log plots:

- Well thicknesses are measured thicknesses, not true vertical thickness.
- The Level of Maturity (LOM) parameter required for the Passey method TOC calculation is assumed to fall within the range chosen (Table 1). Values of LOM outside of this range could change the final TOC value significantly. Sensitivity on this parameter is represented by the blue shading on the log plots and the TOC\_L and TOC\_H values in the tables are based on the values in Table 1. This has significant importance in the region due to the presence of local igneous intrusions which can increase LOM values.
- The Passey method also requires the selection of a 'Lean Shale' point where a shale is assumed to have no organic content or measured TOC wt% values to calibrate the calculations. As there are no notable lean shale intervals in the wells studied, reliance was placed on calibration to measured TOCs. No sensitivity on this parameter has been produced for this study, so this should be taken into consideration when examining the absolute TOC values reported here. For the eastern wells (Carrington 1 and Straiton 1) absolute TOC values should be noted but not relied upon; for these wells the high TOC calculated curve response should be noted, not the TOC values.
- The VCI parameters selected have been chosen as consistently as possible between wells, backed up by neutron-density data where possible to enable distinction between clean and shaly intervals. A cut-off of 0.5 has been arbitrarily applied to remove non-clayey intervals.
- Stratigraphic formation tops for each well were provided from Appendix C.
- The number and location of wells used in this study was limited by the availability of suitable, good quality geophysical log data.

# **4.Results**

Each interval of interest has been assessed and its results reported separately. Comments have been made on the geographical distribution of wells in relation to their TOC values calculated. According to Passey (1990), a mature source rock interval can be distinguished from an immature source rock interval by its increased resistivity. The results for each individual well are reported in the Appendix. These includes graphical log plots, histograms of TOC calculated for each formation and tabulated curve statistics. When assessing the absolute values and quality of the results reported here, the assumptions and limitations (above) should be taken into consideration.

### **Limestone Coal Formation**

The Limestone Coal Formation is on average the richest TOC interval with mean values between 3.9 wt% (*Bargeddie 1*) and 4.3 wt% (*Craighead 1*). Net (shale) thicknesses vary from 20.8 m (*Bargeddie 1*) to 129.9 m (*Craighead1*), with N/G values ranging from 0.97 (*Bargeddie 1*) to 0.38 (*Carrington 1*).

With the cut-offs applied the pay thicknesses vary from 20.8 m (*Bargeddie 1*) to 129.9 m (*Craighead 1*) and pay/gross (P/G) varies from 0.97 (*Bargeddie 1*) to 0.37 (*Carrington 1*).

The reasons for the high variability of the P/G across the 3 wells chosen can be explained when assessing the logs. For *Bargeddie 1* the high P/G is due to the Limestone Coal Formation being incomplete because faulting has removed its upper section. The well has recorded only 20 m of TOC wt% rich shale towards the base of the formation. *Carrington 1* has low P/G because it comprises a relatively clean interval of coals and sands, although more TOC rich shales show towards the base of the formation (as seen in *Bargeddie 1*). *Craighead 1* shows a complete section of interbedded coals, sands and shales at a consistently high TOC. Again the thicker TOC rich shale interval shows towards at the base of the formation.

Regionally, the wells in the west (*Craighead 1* and *Bargeddie 1*) show on average higher TOC wt%, with *Carrington 1* in the east showing a cleaner section with less shale and lower TOC wt%.

	Average TOC	G, Gross	N, Net				P/G for
	over net shale	Formation	(shale)		P, Pay		>15 m
Name	(calculated wt%)	(m)	(m)	N/G	(m)	P/G	snale intervals
Bargeddie 1	2.0	21 5	20.8	0.07	20.8	0.07	1 00
	5.9	21.5	20.8	0.97	20.8	0.97	1.00
Carrington 1	4.0	168.6	64.8	0.38	62.6	0.37	0.00
Craighead 1	4.3	208.5	129.9	0.62	129.9	0.62	0.00
Kelty Bridge 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Straiton 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A

Straiton 1 and Kelty Bridge 1 logs do not record evidence of the Limestone Coal Formation.

**Table 2**: Summary of the average wt% TOC over Net shale thickness, Gross thickness, Net (shale) thickness, Paythickness (for organic-rich shale) and P/G for organic-rich shale intervals >15 m for the lower Limestone Coal Formationacross the analysed wells. Sorted alphabetically. (Note P/G for >15 m shale intervals has a smoothing filter applied,consequently giving higher values than the measured P/G)

#### Lower Limestone Formation

The Lower Limestone Formation is a good source rock interval with mean TOC values between 2.0 wt% (*Carrington 1*) and 3.9 wt% (*Craighead 1*). The net shale thicknesses vary from 43.7 m (*Carrington 1*) to 69.5 m (*Bargeddie 1*), with high N/G values ranging from 0.44 (*Carrington 1*) to 0.74 (*Bargeddie 1*).

With the cut-offs applied the pay thicknesses vary from 24.2 m (*Carrington 1*) to 69.5 m (*Bargeddie 1*) and P/G varies from 0.24 (*Carrington 1*) to 0.74 (*Bargeddie 1*).

There is less variability in the Lower Limestone Formation than the Limestone Coal Formation, although the wells in the west show similar thicknesses, average TOC wt% and P/G. *Carrington 1* in the east shows a similar thickness of formation, but as with the Limestone Coal Formation, the lithologies are cleaner than in the west. P/G values are therefore lower, although a TOC-rich base interval is noticeable.

Straiton 1 and Kelty Bridge 1 logs do not record evidence of the Lower Limestone Formation
	Average TOC over net shale thickness	G, Gross Formation Thickness	N, Net (shale) Thickness		P, Pay Thickness		P/G for >15 m shale
Name	(calculated wt%)	(m)	(m)	N/G	(m)	P/G	intervals
Bargeddie 1	3.4	93.5	69.5	0.74	69.5	0.74	0.65
Carrington 1	2.0	100.0	43.7	0.44	24.2	0.24	0.01
Craighead 1	3.9	91.7	65.5	0.71	64.9	0.71	0.35
Kelty Bridge 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Straiton 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A

**Table 3**: Summary of the average wt% TOC over Net shale thickness, Gross thickness, Net (shale) thickness, Pay thickness (fororganic-rich shale) and P/G for organic-rich shale intervals >15 m for the Lower Limestone Formation in the analysed wells. Sortedalphabetically.

# West Lothian Oil-Shale Formation

The West Lothian Oil-Shale Formation is a fair to good average source rock interval, with mean TOC vales between 1.4 wt% (*Kelty Bridge 1*) and 4.2 wt% (*Craighead 1*). This is the thickest formation with net (shale) thicknesses varying from 105.8 m (*Kelty Bridge 1*) to 284.0 m (*Carrington 1*), with N/G values ranging from 0.37 (*Kelty Bridge 1*) to 0.75 (*Bargeddie 1*).

With the cut-offs applied the pay thicknesses vary from 20.6m (*Kelty Bridge 1*) to 217m (*Craighead 1*) and pay/gross vary from 0.07 (*Kelty Bridge 1*) to 0.72 (*Bargeddie 1*).

*Kelty Bridge 1* proved a relatively thin sequence of the West Lothian Oil-Shale Formation that shows a very clean section with few shale intervals. When the curve was calibrated, the only potential interval of interest was at the top of the logged formation. Furthermore, this well could be underlain by an igneous intrusion (shown by very high R<sub>o</sub> values). The eastern wells (*Craighead 1* and *Bargeddie 1*) are very similar to the western well (*Carrington 1*), showing a variable formation with several intervals of high TOC (denoted by a separation of the scaled sonic and DlogR). For *Carrington 1* these intervals include 975 m, ~1025 m, 1060-1125 m, 1190 m and 1250-1325 m. *Carrington 1* was calibrated to give lower TOC values based on measured TOC values in the nearby *Stewart 1* well (Appendix D), hence many values fall below the 2 wt% TOC cut-off lowering the P/G value.

*Straiton 1* logs do not record evidence of the West Lothian Oil-Shale Formation.

	Average TOC over net shale thickness	G, Gross Formation Thickness	N, Net (shale) Thickness		P, Pay Thickness	- / -	P/G for >15 m shale
Name	(calculated wt%)	(m)	(m)	N/G	(m)	P/G	intervals
Bargeddie 1	2.7	263.0	196.5	0.75	188.9	0.72	0.34
Carrington 1	2.4	491.9	284.0	0.58	154.0	0.31	0.07
Craighead 1	4.2	336.2	222.4	0.66	217.2	0.65	0.32
Kelty Bridge 1	1.4	286.7	105.8	0.37	20.6	0.07	0.00
Straiton 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A

 Table 4: Summary of the average wt% TOC over Net shale thickness, Gross thickness, Net (shale) thickness, Pay thickness (for organic-rich shale intervals >15 m for the West Lothian Oil-Shale Formation across the analysed wells. Sorted alphabetically.

## **Gullane Formation**

The Gullane Formation represents a fair source rock interval with mean TOC values of 2.1 wt% (*Straiton 1*) and 2.2 wt% (*Carrington 1*). Net (shale) thicknesses are 292 m (*Carrington 1*) and 390 m (*Straiton 1*), with N/G values of 0.64 (*Carrington 1*) and 0.84 (*Straiton 1*).

With the cut-offs applied the pay thicknesses vary from 105.6 m (*Carrington 1*) to 134.2 m (*Straiton 1*) and P/G are similar at 0.36 (*Carrington 1*) and 0.34 (*Straiton 1*).

Both *Carrington 1* and *Straiton 1* record a formation with large net shale thickness, although neither has measured TOC values; therefore the calibration and/or LOM affect the calculated TOC curve. The calculated TOC values fall at or just below the 2 wt% TOC cut-off resulting in P/G much lower than the N/G. If the lower maturity value was taken (the upper end of the TOC range represented by blue shading on the graphical logs), the P/G would increase to 0.53 and 0.79 for *Carrington 1* and *Straiton 1* respectively. Above the consistent TOC values are a couple of intervals with higher TOC, for example 1400-1420 m at *Carrington 1*.

*Straiton 1* graphical log shows at least three severe spikes in calculated TOC (410 m, 515-525 m and 550-560 m); these are most likely as a result of the logging. The caliper shows particularly poor hole conditions at the corresponding depths and this is matched by a deviation of the sonic curve. These observations must be taken into consideration when assessing the *Straiton 1* Gullane Formation.

Bargeddie 1, Craighead 1 and Kelty Bridge 1 logs do not record evidence of the Gullane Formation

Name	Average TOC over net shale thickness (calculated wt%)	G, Gross Formation Thickness (m)	N, Net (shale) Thickness (m)	N/G	P, Pay Thickness (m)	P/G	P/G for >15 m shale intervals
Bargeddie 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Carrington 1	2.2	292.0	187.3	0.64	105.6	0.36	0.00
Craighead 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Kelty Bridge 1	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Straiton 1	2.1	390.0	327.3	0.84	134.2	0.34	0.04

**Table 5**: Summary of the average wt% TOC Gross thickness, Net (shale) thickness, Pay thickness (for organic-rich shale) and P/G for organic-rich shale intervals >15 m for the Gullane Formation across the analysed wells. Sorted alphabetically.

# **5.**Conclusions

Geophysical logs from 5 wells across the Midland Valley of Scotland were analysed using the Passey (1990) method for calculating weight percent of Total Organic Content (wt% TOC). The calculations were undertaken for shale intervals in the Carboniferous within the:

- Limestone Coal Formation
- Lower Limestone Formation
- West Lothian Oil-Shale Formation
- Gullane Formation

Where possible, the geographic distribution and trends were examined and commented on. Given the limited availability of data the results show that in the Carboniferous of the Midland Valley of Scotland, not only is there a difference in pay to gross and TOC wt% per formation, but a geographical distinction can also be observed. The geographical distribution shows higher average wt% TOC and P/G in the west (*Craighead 1* and *Bargeddie 1*) in comparison to those in the east, although wells in the east had more limited measured TOC data available for calibration of the log curves.

The Limestone Coal Formation and Lower Limestone Formation show the highest TOC wt% values. The Limestone Coal Formation contains organic rich shales with calculated wt% TOC greater than 2% in both the east and west. The Lower Limestone Formation shows high TOC wt% values. In the east this interval is very similar to the Limestone Coal Formation whereas in the west, this formation has more consistent shale intervals. Both formations have more consistent shale intervals towards their base, with raised TOC.

The West Lothian Oil-Shale Formation is the thickest formation assessed, and shows the greatest variability in TOC wt%. With the exception of *Kelty Bridge 1*, the good P/G and fair average wt% TOC represent a fair to good source rock. Western wells have higher TOC and P/G than those in the east. The West Lothian Oil-Shale Formation contains several intervals with high TOC; these intervals are more discrete in the eastern wells.

The Gullane Formation is only present in two of the eastern wells. It has the poorest average wt% TOC interval and can be said to represent a poor to fair source rock. As with the West Lothian Oil-Shale Formation, high TOC intervals occur. The formation is shale rich with high N/G in both wells, although when the Level of Maturity and calibration estimates are applied, the majority of the values plot lower than 2 wt% TOC, therefore giving a low P/G. A small change in Level of Maturity or calibration could significantly increase the P/G.

The limited availability of data in this study has affected how comprehensively the results can be applied, in particular to the east of the region. In the eastern wells, calibration of the calculated TOC curve was estimated based on measured TOC values from nearby wells. Vitrinite reflectance data had better coverage, but its accuracy is limited. Therefore, the values calculated from eastern wells should be treated with caution, although since the curve shape is correct, intervals of high calculated TOC are representative of in situ raised TOC.

# References

See Main report

# Appendix to well log study

The Level of Organic Maturity (LOM) values are given in Table 1. Average LOM when calculated gives a TOC\_M value; it is represented on the graphical log plots by the pink 'Calculated TOC (wt%)' curve in the right hand column of the log plots below. Minimum and maximum LOMs give TOC\_H and TOC\_L values respectively with a range indicated by blue shading in the right hand column of the graphical log plots below. Each Appendix figure for the wells is accompanied by histograms, TOC statistics and a N/G, P/G summary table. The key to the formations of interest is shown below with the corresponding colours shown on the graphical log plots.



**Figure 1:** A schematic guide for the interpretation of a variety of features seen on the  $\Delta \log R$  overlays. The part relating to distinguishing the maturity of source shale rock for this study is highlighted (modified from Passey *et al.* 1990).

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Figure 2: Bargeddie 1





Figure 2a: TOC histograms by formation. The calculated TOC\_M curve with VCL cut-off of 0.5 has been applied.

Curve	Min	Max	Mean									
Limestone Coal Formation												
TOC_M	2.2	7.2	3.9									
TOC_L	1.9	5.6	3.2									
ТОС_Н	2.7	9.4	5.0									
Lower Limestone Formation												
TOC_M	2.7	5.7	3.4									
TOC_L	2.2	4.5	2.7									
ТОС_Н	3.4	7.4	4.2									
West Lothian Oil-S	hale Forr	mation										
TOC_M	1.9	6.2	2.7									
TOC_L	1.7	5.2	2.4									
ТОС_Н	2.1	7.3	3.2									

# Table 2a (Left):

Summary statistics for calculated TOC wt% by formation.

- TOC\_M: Calculated TOC wt% based on the Passey-Sonic method using an average LOM
- TOC\_L and TOC\_H: Calculated range of TOC wt% with high and low LOM (graphically represented by the blue shading)

	Тор		Gross	Net (shale)		Рау		Рау		Рау		P/G shale
	Depth	Bottom	Formation	Thickness		Thickness	P/G	Thickness	P/G	Thickness	P/G	intervals
Zone	(m)	Depth (m)	Thickness (m)	(m)	N/G	(тос_м)	(TOC_M)	(TOC_L)	(TOC_L)	(тос_н)	(тос_н)	>15 m
Limestone Coal Fm	665.0	686.5	21.5	20.8	0.97	20.8	0.97	20.6	0.96	20.8	0.97	1.00
Lower Limestone Fm	686.5	780.0	93.5	69.5	0.74	69.5	0.74	69.5	0.74	69.5	0.74	0.34
West Lothian Oil-												0.65
Shale Fm	780.0	1043.0	263.0	196.5	0.75	188.9	0.72	166.9	0.64	190.5	0.72	
All Zones	665.0	1043.0	378.0	286.8	0.76	279.2	0.74	257.0	0.68	280.8	0.74	0.66

Figure 3: Carrington 1 Carrington NT36SW/259 Scale : 1 : 5000 DB : DECC (30) DEPTH (600M - 1700.02M) Depth (M) FΜ Volume of Clay (Dec) DTovl (uSec/ft) Caliper (IN) - 16. 0. -1. -1. 3. 0. 4. LogRT ()







Figure 3a: TOC histograms by formation	<ol> <li>The calculated TOC_M curve with VCL cut-off of 0.5 has</li> </ol>
been applied.	

Curve	Min	Max	Mean							
Limestone Coal Formation										
TOC_M	0.0	8.5	4.0							
TOC_L	0.0	6.9	3.3							
TOC_H	0.0	12.2	5.5							
Lower Lim	estone Fo	ormation	1							
TOC_M	0.0	5.1	2.0							
TOC_L	0.0	4.2	1.8							
TOC_H	0.0	7.2	2.7							
West Lothia	an Oil-Shal	e Formati	ion							
TOC_M	0.0	10.1	2.4							
TOC_L	0.0	8.4	2.1							
TOC_H	0.0	14.5	3.1							
Gullane Fo	ormation									
TOC_M	0.0	6.9	2.2							
TOC_L	0.0	5.5	1.9							
TOC_H	0.0	10.8	3.2							

### Table 3a (Left):

•

Summary statistics for calculated TOC wt% by formation.

- TOC\_M: Calculated TOC wt% based on the Passey-Sonic method using an average LOM
  - TOC\_L and TOC\_H: Calculated range of TOC wt% with high and low LOM (graphically represented by the blue shading)

## Table 3b (Below):

Summarising each formation's Net to Gross (N/G), Pay to Gross (P/G), P/G for the TOC wt% range (TOC\_L and TOC\_H) and P/G for organic-rich shale intervals >15 m (50 ft). Summation of all zones of interest is included.

			Gross									P/G
	Тор	Bottom	Formation	Net (shale)		Рау				Рау		shale
	Depth	Depth	Thickness	Thickness		Thickness	P/G	Pay Thickness	P/G	Thickness	P/G	intervals
Zone	(m)	(m)	(m)	(m)	N/G	(TOC_M)	(TOC_M)	(TOC_L)	(TOC_L)	(TOC_H)	(TOC_H)	>15 m
Limestone Coal Fm	627.6	796.1	168.6	64.8	0.38	62.6	0.37	62.9	0.37	62.2	0.37	0.00
Lower Limestone Fm	796.1	896.1	100.0	43.7	0.44	24.2	0.24	29.9	0.30	15.2	0.15	0.07
West Lothian Oil-Shale												0.01
Formation	896.1	1388.0	491.9	284.0	0.58	154.0	0.31	200.3	0.41	127.8	0.26	
<b>Gullane Formation</b>	1388.0	1680.0	292.0	187.3	0.64	105.6	0.36	154.7	0.53	67.7	0.23	0.00
All Zones	627.6	1680.0	1052.4	579.8	0.55	346.4	0.33	447.9	0.43	272.8	0.26	0.02

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Figure 4: Craighead 1



Figure 4a: TOC histograms by formation. The calculated TOC\_M curve with VCL cut-off of 0.5 has been applied.

Curve Limeston	Min M e Coal Forma	ax tion	Mean	Table 4a (	Left):								
TOC_M	2.7	6.4	4.3	Summary	statistics for	r calcula	ted TOC wt	% by forma	tion.				
TOC_L	2.2	5.0	) 3.4										
тос_н	3.4	8.3	3 5.4	• TC	DC_M: Calcu	lated T	OC wt% bas	ed on the P	assey-Sonic ı	method us	sing an aver	age LOM	
Lower Lin	nestone Form	nation		• TC	C L and TC	C H: Ca	alculated rai	nge of TOC	wt% with hig	h and low	I OM (gran	hically rep	resented by the
TOC_M	1.4	4.9	3.9	. e	oding)						2011 (Brap	incany rep	
TOC_L	1.3	3.9	) 3.1	SII	aung								
тос_н	1.7	6.3	3 4.9	Table 4h (	Below):								
West Loth	ian Oil-Shale F	ormation											
TOC_M	0.0	13.6	5 4.2	Summarisi	ing each for	mation'	s Net to Gro	oss (N/G). P	av to Gross (I	P/G) P/G	for the TOC	wt% rang	e (TOC L and
TOC_L	0.0	11.3	3.6										
TOC_H	0.0	16.3	3 4.9	TOC_H) ar	id P/G for o	rganic-ri	ich shale int	ervais > 15	m (50 ft). Su	mmation	or all zones	or interes	is included.
				Gross	Net								
		Тор		Formation	(shale)		Рау		Рау		Рау		P/G shale
		Depth	Bottom	Thickness	Thickness		Thickness	P/G	Thickness	P/G	Thickness	P/G	intervals
Zone		(m)	Depth (m)	(m)	(m)	N/G	(TOC_M)	(TOC_M)	(TOC_L)	(TOC_L)	(тос_н)	(TOC_H)	>15 m
Limeston	e Coal Fm	263.6	472.1	208.5	129.9	0.62	129.9	0.62	129.9	0.62	129.9	0.62	0.00
Lower Lin	nestone Fm	472.1	563.8	91.7	65.5	0.71	64.9	0.71	64.3	0.70	65.2	0.71	0.32
West Lothia	n Oil-Shale Fm	563.8	900.0	336.2	222.4	0.66	217.2	0.65	216.9	0.65	217.5	0.65	0.35
<b>All Zones</b>		263.6	900.0	636.4	417.7	0.66	411.9	0.65	411.0	0.65	412.5	0.65	0.34

- e blue







WLO TOC wt%

**Figure 5a:** TOC histogram of the West Lothian Oil-Shale Formation. The calculated TOC\_M curve with VCL cut-off of 0.5 has been applied.

#### Table 5a (Left):

Curve	Min	Max	Mean
West Lothi	an Oil-Sha	le Format	ion
TOC_M	0.0	6.0	1.4
TOC_L	0.0	4.5	1.2
TOCH	0.0	7.7	1.6

Summary statistics for calculated TOC wt% for the West Lothian Oil-Shale Formation.

- TOC\_M: Calculated TOC wt% based on the Passey-Sonic method using an average LOM
- TOC\_L and TOC\_H: Calculated range of TOC wt% with high and low LOM (graphically represented by the blue shading)

### Table 5b (Below):

Summarising the West Lothian Oil-Shale Formation's Net to Gross (N/G), Pay to Gross (P/G), P/G for the TOC wt% range (TOC\_L and TOC\_H) and P/G for organic-rich shale intervals >15 m (50 ft).

			Gross	Net								
	Тор		Formation	(shale)		Pay		Рау				P/G shale
	Depth	Bottom	Thickness	Thickness		Thickness	P/G	Thickness	P/G	Pay Thickness		intervals
Zone	(m)	Depth (m)	(m)	(m)	N/G	(тос_м)	(TOC_M)	(TOC_L)	(TOC_L)	(TOC_H)	P/G (TOC_H)	>15 m
West												0.00
Lothian												
Oil-Shale												
Fm	155.0	441.7	286.7	105.8	0.37	20.6	0.07	32.0	0.11	10.5	0.04	

APPENDIX F TO 'THE CARBONIFEROUS SHALES OF THE MIDLAND VALLEY OF SCOTLAND: GEOLOGY AND RESOURCE ESTIMATION'



Straiton 1 NT26NE/291 DECC:TOC\_DLRS (wt%) 100 1050 90 900 80 Cumulative Frequency 70 750 Number of Points 60 600 50 450 40 30 300 20 150 10 -+0 10 앙 4 5 9 1 2 3 6 7 8 3273 points plotted out of 3901 (Discriminators applied) Curve Zone Depths DECC:TOC\_D (1) Gullane 250M - 640M WLO TOC wt%

**Figure 6a:** TOC histogram of the Gullane Formation. The calculated TOC\_M curve with VCL cutoff of 0.5 has been applied.

#### Table 6a (Left):

Curve	Min	Max	Mean
Gullane F	ormatio	n	
TOC_M	0.0	8.3	2.1
TOC_L	0.2	6.3	1.8
TOC_H	0.0	13.7	3.0

Summary statistics for calculated TOC wt% for the Gullane Formation.

- TOC\_M: Calculated TOC wt% based on the Passey-Sonic method using an average LOM
- TOC\_L and TOC\_H: Calculated range of TOC wt% with high and low LOM (graphically represented by the blue shading)

#### Table 6b (Below):

Summarising the Gullane Formation's Net to Gross (N/G), Pay to Gross (P/G), P/G for the TOC wt% range (TOC\_L and TOC\_H) and P/G for organic-rich shale intervals >15 m (50 ft).

	Gross							
Bottom	Formation	Net (shale)	Pav	Pav	Pav	shale		

	Top Depth	Depth	Thickness	Thickness		Thickness	P/G	Thickness	P/G	Thickness	P/G	intervals
Zone	(m)	(m)	(m)	(m)	N/G	(TOC_M)	(TOC_M)	(TOC_L)	(TOC_L)	(ТОС_Н)	(TOC_H)	>15 m
<b>Gullane Formation</b>	250.0	640.0	390.0	327.3	0.84	134.2	0.34	305.1	0.78	60.8	0.16	0.04