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GEOLOGICAL SURVEY OF CANADA
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Abstract

Exploration of conventional/unconventional hydrocarbon resources relies on detailed analysis of source/reservoir rocks. Rock-Eval® analysis is one of the major methods in screening and characterizing the organic matter type and quantity, thermal maturity, and hydrocarbon potential of sedimentary rocks (Lafargue et al., 1998). In addition, Rock-Eval® analysis is also widely used for characterization of organic matter in recent sediments and soil in wide range of environmental and soil fertility studies (e.g., Sanei et al., 2005; Carrie et al., 2012). Fundamentals of Rock-Eval® analysis are provided in detail in Lafargue et al. (1998) and Behar et al. (2001).

In order to determine the accuracy and precision of analysis, a formally certified standard reference material is typically analysed concurrently with samples to assure the consistency of measured data. However, no commercially available certified reference materials have been characterized for the parameters measured during Rock-Eval® analysis. Instead, the Geological Survey of Canada (GSC) Organic Geochemistry Laboratory uses an internal prepared standard (9107) that was calibrated against a rock standard provided by the instrument manufacturer. That standard was developed by using various gravimetric approaches and external calibration of the Rock-Eval flame ionization (hydrocarbons) and thermal conductivity or infrared (CO and CO_2) detectors. The 9107 standard is from the Upper Cretaceous Second White Speckled Shale, Colorado Group in western Canada, which is regarded as a typical marine hydrocarbon source rock. This standard is run in a sample batch of 10 to 15 unknown samples to verify the analytical performance of Rock-Eval® instrument and ensure the consistency of generated data throughout series of analyses.

This report presents the summary results of more than 2000 runs of the 9107 standard since the deployment of three completely refurbished Rock-Eval 6® instruments at the GSC in 2007documenting the accepted values of selected measured Rock-Eval 6® parameters and measurement precision and margin of error for the 9107 standard.

Method

The 9107 standard is a calcareous marine organic rich shale sample from the Upper Cretaceous Second White Speckled Shale of the Colorado Group. This sample was collected in an outcrop from a 10-15 cm thick massive homogeneous bed of the formation in Sheep River valley south Okotoks, Alberta. The standard sample was excavated from several centimeters below the surface of the outcrop to avoid effects of weathering. Several kilograms of unaltered rock material were air dried at room temperatures, crushed with a disk mill and then pulverized in a swing mill and mixed to obtain a homogeneous sample that has been used as the Rock-Eval

standard at the GSC Calgary since 1991. The original calibration of the 9107 standard was carried out using a standard rock material that had been provided by the Institut Français du Pétrole (IFP) when the instruments were purchased.
We synthesized the Rock-Eval 6® data for 2151 analysis of 9107 standard carried out between 2007 to 2015 in the Organic Geochemistry and Petrology Laboratory of the Geological Survey of Canada, Calgary. During this period, all three Rock-Eval 6® instruments were operated in optimal condition. We screened the data to remove any possible entry affected by analysis failures such as a misidentified sample, hardware malfunction, mechanical failure of the sample handling robot and/or gas supply failure. To exclude measurement outliers, the 95% percentile of values was selected as the cut-off. The median values of the resulting cleaned dataset (N = 2151) were used to exclude any influence of any remaining outliers due to natural fluctuations in analysis and/or possible natural heterogeneity of the standard sample. The resulting median values shown in Table 1 represent statistically valid, accepted values for the 9107 GSC internal standard.
The error for the majority of measured parameters except S3 and S3CO are less than 10% (Table 1).The relatively lower precision for the S3 in bulk samples is expected and is often due to poor peak integration and distinction between S3 organic matter and S3 carbonates (derived from the presence of siderite in the samples). Decarbonization of the samples is expected to improve the precision of S3 measurement. The poor precision for S3CO is due to low detection in the standard shale.

Conclusion

This document reports the accepted Rock-Eval 6® values for GSC internal standard 9107 (Second White Speckled Shale of the Colorado Group). The accepted values for N=2151 measurements are:

S1	S2	S3	T_{max}	T_{peak}	S3CO	PC	TOC	RC	HI	OI	PI	MINC	OICO	S4CO	$S4CO_2$
mg HC/g rock	mg HC/g rock	mg CO_2/g rock	°C	°C	mg CO/g rock	wt. %	wt. %	wt. %	mg HC/g TOC	mg CO_2/g TOC	-	wt. %	mg CO/g TOC	mg CO/g rock	mg CO_2/g rock
0.72	12.18	0.55	442	481	0.17	1.10	5.07	3.97	240.16	10.87	0.06	4.20	3.00	22.01	111.58

These values are recommended for data quality control and quality assurance of GSC Rock-Eval analyses.

References

Behar, F., Beaumont, V., De, B., Penteado, H.L., 2001. Rock-Eval 6 technology: performances and developments. Oil Gas Sci. Technol. Rev. IFP 56, 111–134.

Carrie, J., Sanei, H., Stern, G. 2012. Standardisation of Rock–Eval pyrolysis for the analysis of recent sediments and soils. Organic Geochemistry 46, 38-53.

Lafargue, E., Espitalié, J., Marquis, F., Pillot, D., 1998. Rock-Eval 6 applications in hydrocarbon exploration, production and soil contamination studies. Revue de l'Institut Français du Pétrole 53, 421–437.

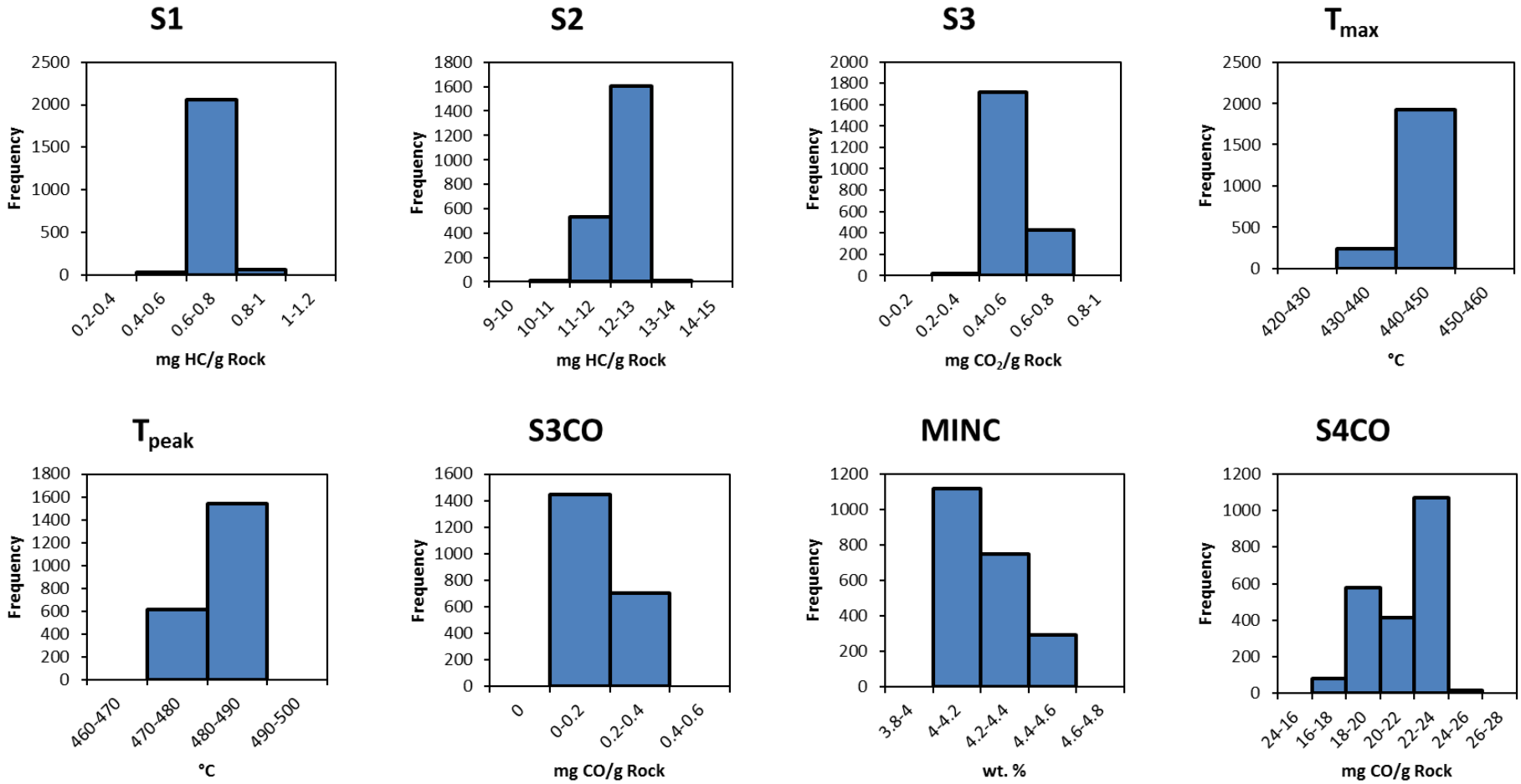
Sanei, H., Stasiuk, L.D., Goodarzi, F. 2005. Petrological changes occurring in organic matter from recent lacustrine sediments during thermal alteration by Rock-Eval pyrolysis. Organic Geochemistry 36, 1190-1203.

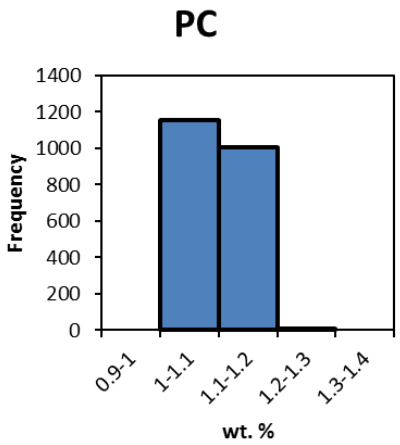
Table 1.Summary statistics of measured Rock-Eval 6® parameters and their accepted values for 9107 internal standard.

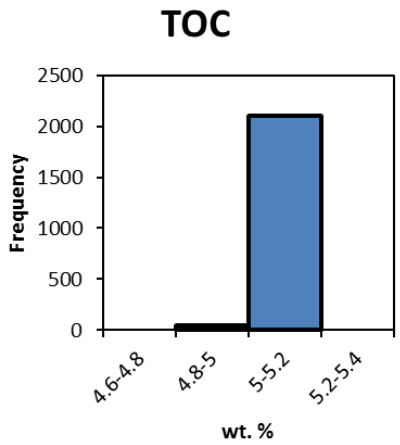
	^{1}S1	^{2}S2	^{3}S3	$^{4}T_{max}$	$^{5}T_{peak}$	^{6}S3CO	^{7}PC	^{8}TOC	^{9}RC	^{10}HI	^{11}OI	^{12}PI	^{13}MINC	^{14}OICO	^{15}S4CO	$^{16}S4CO_2$
	mg HC/g rock	mg HC/g rock	mg CO_2/g rock	°C	°C	mg CO/g rock	wt. %	wt. %	wt. %	mg HC/g TOC	mg CO_2/g TOC	-	wt. %	mg CO/g TOC	mg CO/g rock	mg CO_2/g rock
n	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151	2151
mean	0.72	12.17	0.55	441.77	480.90	0.17	1.10	5.07	3.97	239.97	10.82	0.06	4.24	3.33	21.28	112.14
median	0.72	12.18	0.55	442.00	481.00	0.17	1.10	5.07	3.97	240.16	10.87	0.06	4.20	3.00	22.01	111.58
stdev.	0.04	0.28	0.06	1.05	1.26	0.07	0.02	0.04	0.04	5.57	1.15	0.00	0.11	1.48	1.76	2.79
max	0.98	13.36	0.66	448.00	487.00	0.34	1.21	5.14	4.10	260.74	13.20	0.07	4.48	7.00	25.01	123.46
min	0.48	11.00	0.40	437.00	476.00	0.05	1.01	5.00	3.82	216.83	7.83	0.04	4.07	1.00	16.10	105.90
error	**6%**	**2%**	**11%**	**0%**	**0%**	**43%**	**2%**	**1%**	**1%**	**2%**	**11%**	**5%**	**3%**	**45%**	**8%**	**2%**
accepted value	**0.72**	**12.18**	**0.55**	**442.00**	**481.00**	**0.17**	**1.10**	**5.07**	**3.97**	**240.16**	**10.87**	**0.06**	**4.20**	**3.00**	**22.01**	**111.58**

^{1}S1: Free hydrocarbon; ^{2}S2: Kerogen/Remaining hydrocarbon potential; ^{3}S3: CO_2 from cracking of organic matter; $^{4}T_{max}$: Pyrolysis temperature; $^{5}T_{peak}$: True pyrolysis temperature; ^{6}S3CO: CO from pyrolysis; ^{7}PC: Pyrolyzed carbon; ^{8}TOC: Total organic carbon; ^{9}RC: Residual carbon; ^{10}HI: Hydrogen index; ^{11}OI: Oxygen Index; ^{12}PI: Production index; ^{13}MINC: Mineral carbon; ^{14}OICO: CO oxygen index; ^{15}S4CO: CO from oxidation; $^{16}S4CO_2$: CO_2 from oxidation.

Figure 1.Histograms of measured and calculated Rock-Eval 6® parameters for 9107 internal standard for 2151 samples.




PC
Frequency
1400
1200
1000
800
600
400
200
0
0.9-1
1-1.1
1.1-1.2
1.2-1.3
1.3-1.4
wt. %


TOC
Frequency
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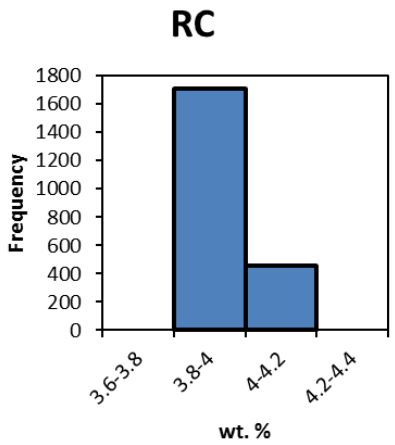
2000
1500
1000
500
0
4.6-4.8
4.8-5
5-5.2
5.2-5.4
wt. %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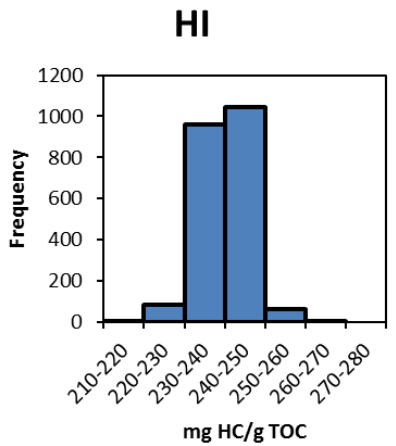
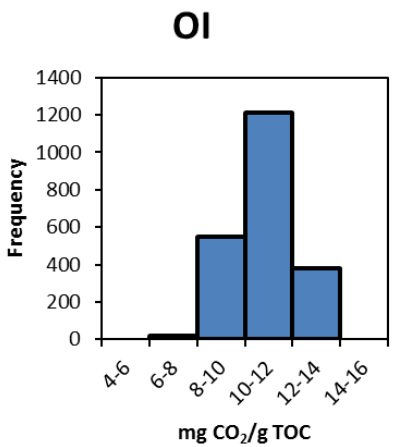
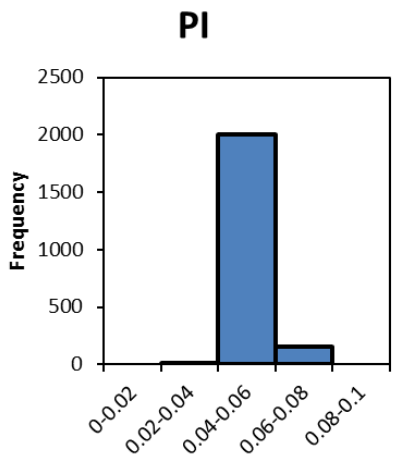
Frequency
1800
1600
1400
1200
1000
800
600
400
200
0
3.6-3.8
3.8-4
4-4.2
4.2-4.4
wt. %


HI
Frequency
1200
1000
800
600
400
200
0
210-220
220-230
230-240
240-250
250-260
260-270
270-280
mg HC/g TOC


OI
Frequency
1400
1200
1000
800
600
400
200
0
4-6
6-8
8-10
10-12
12-14
14-16
mg CO2/g TOC


PI
Frequency
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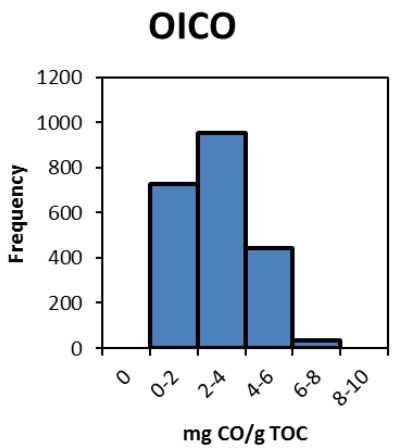
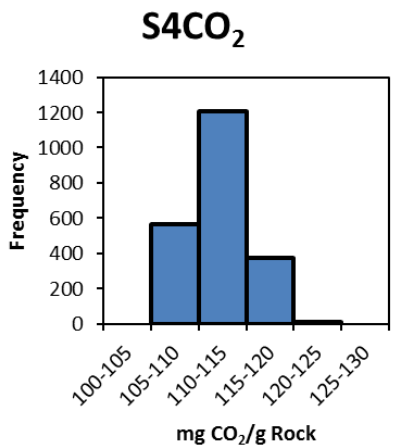
2000
1500
1000
500
0
0-0.02
0.02-0.04
0.04-0.06
0.06-0.08
0.08-0.1


OICO
Frequency
1200
1000
800
600
400
200
0
0
0-2
2-4
4-6
6-8
8-10
mg CO/g TOC


S4CO2
Frequency
1400
1200
1000
800
600
400
200
0
100-105
105-110
110-115
115-120
120-125
125-130
mg CO2/g Rock