
Source Rock (SR) Analyzer: User Guide

Manual Information

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Introduction

This user guide contains standard operational procedures for the Source Rock Analyzer (SRA). The chemistry laboratory technician performs maintenance and configuration of the SRA. Information for the laboratory technician is presented in the *SRA Analyzer Advanced User Guide*.

Method Overview

Pyrolysis analysis is conducted on dried and ground sediments or borehole source rock for the purpose of safety monitoring. The analysis yields information about thermal maturation and source of hydrocarbons at the drilled site, as well as petroleum potential.

Method Theory

The pyrolysis method consists of a programmed temperature heating in a pyrolysis oven in an inert atmosphere (helium) of a small sample (~50–100 mg) to quantitatively and selectively determine free hydrocarbons contained in the sample and the hydrocarbon- and oxygen-containing compounds that are volatilized during the cracking of unextractable organic matter in the sample (kerogen).

- Free hydrocarbons volatilized below 330°C and measured by the flame ionization detector (FID) comprise the S1 peak.
- Very heavy hydrocarbons (>C₄₀) volatilize and nonvolatile organic compounds crack at temperatures up to 550°C. These are measured by FID and comprise the S2 peak.
- CO₂ released during kerogen cracking in the 300°–390°C range is measured on an infrared detector (S3 peak).

Maturation of organic matter can be estimated by the T_{max} range:

- $T_{max} = 400^{\circ}\text{--}430^{\circ}\text{C}$: immature organic matter
- $T_{max} = 435^{\circ}\text{--}450^{\circ}\text{C}$: mature or oil zone
- $T_{max} > 450^{\circ}\text{C}$: overmature zone

Pyrolysis data may be compromised in samples containing >10 wt% carbonate and for young (<1 Ma) or very immature organic matter ($T_{max} < 400^{\circ}\text{C}$) (Peters, 1986). Samples with <0.5 wt% TOC may not give reliable results because of the small size of the S1, S2, and S3 signals.

Data Values

The data obtained from the Rock-Eval/TOC analyses are defined by the following parameters (Espitalié et al., 1977):

- S1, S2, S3, S4
- Tmax
- Total Organic Carbon (TOC)
- Hydrocarbon Index (HI)
- Oxygen Index (OI)
- Production Index (PI)
- S1/TOC
- Pyrolysis Carbon (PC)
- Residual Carbon (RC)
- S2/S3

S1 Parameter

S1 (milligrams of hydrocarbon per gram of rock) is an indication of free hydrocarbons (gas and oil) in the sample. S1 > 1 mg HC/g rock may be indicative of an oil show. S1 normally increases with depth.

Free thermally extractable hydrocarbons in the whole rock sample that vaporize at temperatures up to ~330°C are included in S1. Heavier free hydrocarbons and nonhydrocarbons (resins, asphaltenes) that vaporize or crack at higher temperatures are included in the S2 peak (Clementz, 1979). Determination of the total thermal extractable content (S1) in some cases may require analysis of extracted rock samples that add the reduction in S2 (S2 whole rock – S2 extracted rock) to the whole rock S1 to account for the heavy free hydrocarbons that carry over into the S2 peak.

S1 can be elevated by contamination from organic drilling fluid additives such as diesel, walnut shells, Qwik-Seal, Lubra beads, gilsonite, etc. Nonindigenous hydrocarbons expelled from source rocks elevate the S1 value in a res-

ervoir rock. Also, fungi growth on wet samples increase S1 (Peters, 1986). Ratios (PI, S1/TOC) are increased as a result of any of these factors.

To convert S1 from mg HC/g rock to ppm, multiply the S1 value by 1000. To convert the original S1 value to an approximate barrels of oil per acre foot, multiply by 20.082.

$$(\text{mg HC/g}) \times (20.082 \text{ bbl}\cdot\text{g}/\text{acre}\cdot\text{ft mg HC}) = \text{bbl}/\text{acre ft}$$

S2 Parameter

S2 (milligrams of hydrocarbon per gram of rock) hydrocarbons result from the cracking of kerogen and high molecular weight free hydrocarbons that do not vaporize in the S1 peak. S2 is an indication of the quantity of hydrocarbons that the rock has the potential of producing should burial and maturation continue. This parameter normally decreases with burial depths >1 km. The shape of the S2 peak is characteristic of the organic matter type.

S2 values may be reduced by weathering effects, as atomic H/C ratios are reduced by oxidation (van Krevelen, 1984). Also, S2 values may be affected by salt ionization due to saltwater/mineral decomposition at very high temperatures (>550°C) or a high FID/splitter block temperature on the pyrolysis instrument (Espitalié et al., 1985).

To convert to ppm, multiply the S2 value by 1000. To convert the original S2 value to an approximate barrels of oil per acre foot, multiply by 20.082.

T_{max} (°C) Parameter

T_{max} = temperature of maximum rate of evolution of S2 hydrocarbons (top of S2 peak). T_{max} indicates the stage of maturation of the organic matter. T_{max} values are affected by low organic matter content where low S2 peaks are encountered. When the S2 value is <0.5 mg HC/g rock and the S2 peak does not have a definitive peak (i.e., is broad and flat), T_{max} values may not be reliable. Also, organic-lean clayey sediments with S2 values as high as 2.00 mg HC/g rock may have unreliable T_{max} values (Espitalié et al., 1985).

T_{max} may be affected by the presence of heavy free hydrocarbons in the S2 peak, which may cause T_{max} to be anomalously low (<400°C). Also, T_{max} may be affected by reworked organic matter or salt ionization, which may cause T_{max} to be anomalously high (>550°C).

T_{max} values and true T_{max} temperatures vary with the temperature programming rate (Claypool and Reed, 1976) and are useful for approximating kinetic values. T_{max} is a calibrated temperature and does not represent the true (absolute) temperature.

S3 Parameter

S3 (milligrams of organic carbon dioxide per gram of rock) is produced during pyrolysis of kerogen and is organic carbon dioxide evolved during low-temperature pyrolysis (<390°C nominal). It may be affected by the decomposition of inorganic matrix particularly due to weathering or mineral matrix interaction. Generally, S3 values >200 mg CO₂/g rock are anomalously high, possibly due to high concentrations of carbonates that break down at temperatures <390°C and may or may not be valid. S3 is an indication of the amount of oxygen in the kerogen and is used to calculate the oxygen index [see [Oxygen Index \(OI\) Parameter](#)].

S4 Parameter

S4 (milligrams of carbon per gram of rock) is obtained from oxidizing (at 600°C) the organic matter remaining in the sample after pyrolysis (residual carbon). Using this value, TOC is determined by adding the residual organic carbon to the pyrolyzed organic carbon. Because the instrument automatically combines convertible carbon (pyrolyzed carbon) with the residual carbon (RC) and reports TOC to actually determine the S4 value, it is necessary to subtract the convertible carbon from the TOC.

$$S4 = 10 \times \text{TOC} - [0.83 \times (S1 + S2)]; \text{RC} = S4/10$$

TOC Parameter

TOC = weight percent of carbon (unit weight of carbon per unit weight of whole rock). TOC is composed of convertible fraction, which represents the hydrocarbon already generated (S1) and the potential to generate hydro-

carbons (S2). The residual fraction (S4) has no potential to generate hydrocarbons. In Rock-Eval terms the TOC is defined as:

$$\text{TOC} = \text{PC} + \text{RC}$$

$$\text{TOC} = [k \times (S1 + S2)]/10 + S4/10$$

Where PC = pyrolyzed carbon and RC = residual carbon. $k = 83$ (an average carbon content of hydrocarbons by atomic weight); for inertinitic-rich samples, the k value may be as high as 89.

Hydrocarbon Index (HI) Parameter

HI = normalized hydrocarbon content of a rock sample. Kerogen type information is derived from this value as follows:

- Type I kerogens are hydrogen rich
- Type III kerogens are hydrogen poor
- Type II kerogens are intermediate between Type I and Type III

HI decreases as the sample matures. HI may be lowered by weathering or mineral matrix interactions, which cause reduction in the S2 value. Marine organisms and algae, in general, are composed of lipid- and protein-rich organic matter, where the ratio of H to C is higher than in the carbohydrate-rich constituents of land plants. HI typically ranges from ~100 to 600 in geological samples. High HI values (>400) indicate large proportions of well-preserved algal and microbial organic matter.

$$\text{HI} = (S2 \times 100)/\text{TOC}$$

Oxygen Index (OI) Parameter

OI = normalized oxygen content of a rock sample. Type III kerogens generally have higher OI than either Type I or II kerogens. However, the hydrogen content is the principal discriminating factor for oil or gas potential. OI may be increased by weathering or mineral matrix interactions, which elevate the S3 value. If TOC is <0.50 wt%, OI may be meaningless (Espitalié, 1982). OI correlates with the ratio of O to C, which is high for polysaccharide-rich remains of land plants and inert organic material encountered as background in marine sediments. OI values range from near 0 to ~150. High OI values (>100) are an indicator of continental organic matter or immature organic matter from all sources.

$$\text{OI} = (S3 \times 100)/\text{TOC}$$

Production Index (PI) Parameter

PI (Espitalié et al., 1977) is indicative of the conversion of kerogen into free hydrocarbons or, in a general sense, the transformation ratio. PI increases with increasing thermal maturation in the absence of expulsion. Anomalies may be due to differences in organic facies or migration into or expulsion out of a sediment sample. PI values indicate the following:

- $\text{PI} < 0.2$: immature rocks
- $\text{PI} = 0.3\text{--}0.4$: typical for samples in the petroleum window
- $\text{PI} > 0.5$: may indicate proximity of migrated hydrocarbons or trapped petroleum

$$\text{PI} = [S1/(S1 + S2)] \times 100$$

S1/TOC Parameter

The ratio of free hydrocarbons (S1) to TOC may be used to identify source or reservoir rocks (Jarvie and Baker, 1984). The S1 determination yields lighter hydrocarbons, which are usually lost during solvent evaporation. Solvent extraction is much more complete in the nonhydrocarbon (NSO and asphaltene) fraction. This parameter can be evaluated as follows:

- Source rocks have above average S1/TOC ratios

- Reservoir rocks have very high S1/TOC ratios

Evaluation requires assessment of possible contamination by drilling fluid additives and regional geochemistry of sediments.

$$S1 \times 100/TOC$$

Pyrolysis Carbon (PC)

PC (Espitalié, 1982) represents the carbon content of the free hydrocarbons generated ($0.083 \times S1$) plus the carbon content in the remaining potential hydrocarbons ($0.083 \times S2$). In immature samples S2 predominates (excluding reservoir rocks), whereas in postmature rocks the S1 predominates:

- PC > 30%: oil-prone source rock
- PC < 30%: gas-prone source rock

$$PC = 0.83 \times (S1 + S2)/10$$

Residual Carbon (RC)

RC represents the carbon present in kerogen, which has very low potential to generate hydrocarbons. The residual carbon percentage of the TOC increases with kerogen type in the order III > II > I. RC remains relatively constant at any given maturity for Type II and III source rocks.

$$RC = S4/10$$

S2/S3

The S2/S3 ratio was utilized by Clementz et al. (1979) as an indication of kerogen type in the absence of TOC data. This ratio reflects the ratio of hydrogen to oxygen, which is similar to HI divided by OI.

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Apparatus, Reagents, & Materials

SRA Hardware

The SRA system consists of the following main components (**Figure 1**):

- Autosampler

- Main control unit: oven and detector temperature control unit and gas flow controllers for the FID combustion gas, carrier gas, and oxidation gas
- Infrared (IR) section
- Combustion with gas separation and FID (pedestal, oven, and conversion FID)



Figure 1. Four Main Components of the SRA System.

Dual Balance System

Hardware

A Cahn electrobalance is used to measure the mass of samples for the SR Analyzer (*Figure 2*).



Figure 2. Cahn Electrobalance.

Dual Balance System Software

Motion compensation software allows the user to weigh the mass of chemicals and samples at sea (*Figure 3*).

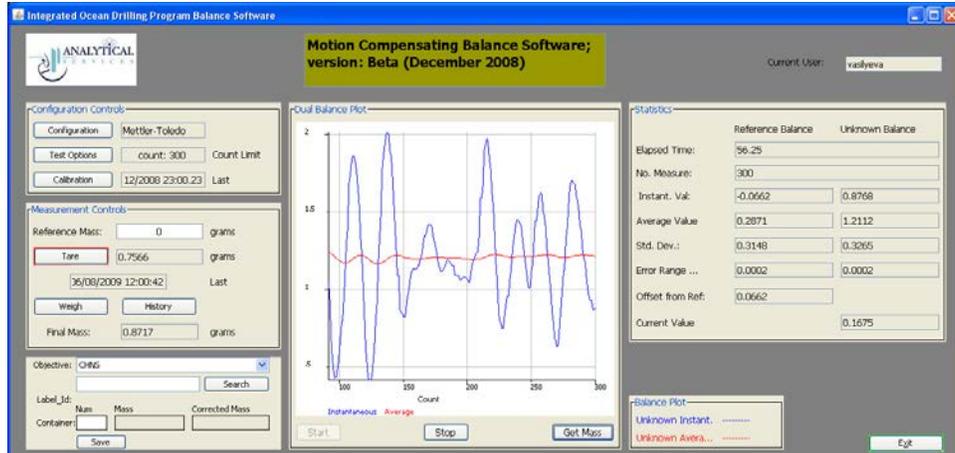


Figure 3. Dual Balance Control Software Main Screen.

Laboratory Equipment

- Analytical balance (see Figure 2; Analytical Balance User Guide)
- SR Analyzer, Humble Instruments and Services

Laboratory Apparatus for Sample Preparation

- Autosampler tray (1/4)
- Forceps
- Small spatula
- Sample filler
- Crucible and crucible holder
- Weighing paper
- Recording chart



Figure 4. SRA Sample Preparation Tools.

Reagents

- Methanol
- Compressed gases
 - Hydrogen, 60–80 psi (4–5.5 bar)
 - Helium carrier gas, 60–80 psi (4–4.5 bar)
 - Air, GC analysis grade, 60–80 psi (4–4.5 bar)
 - Air, laboratory grade, 60–100 psi (4–6.8 bar)

Standards

- Colorado Oil Shale Silica (COSS) house standard
- Standard material (99986)

Instrument Calibration

The first sequence for an expedition must include a Blank and a Standard to calibrate the SRA each time the instrument is turned on after power off (e.g., loss of power). After this initial calibration, a Blank and a Standard should be measured once per day to verify calibration of the SRA.

If one calibration applies to several batches, each batch should include a QA/QC Standard to verify calibration.

See the *SR Analyzer Advanced User Guide* for information about calibrating the detectors.

Sample Preparation

Sediments and sedimentary rock samples logged into the LIMS system as **SRANL** are analyzed by SRA. During sample preparation, keep in mind that sample container numbers must correlate with autosampler place numbers.

Sample preparation includes the following steps:

- Freeze-dry sample
- Grind and homogenize sample
- Weigh sample
- Place sample in a crucible in the autosampler tray

Drying and Grinding Samples

1. Obtain freeze-dried bulk sample (sediments, sedimentary rock, etc.).
2. Crush sample by hand or use an electric mill to roughly crush samples.
3. Homogenize sample using a mortar and pestle. **Note:** Inadequate homogenization will cause high standard deviation in the data.

Text ID (parent)	Text ID (child)	Mass	Container number	LIMS code	SRA code
Blank			99 (Calibration blank; always 99)		BLK
STD99986	OTHR137987	65.0	100 (Calibration STD; always 100)	QAQCSTD	STD
OTHR2764599	OTHR346972	78.26	1	UNK	TPH
OTHR2765092	OTHR130746	70.63	2	UNK	TPH
:	:	:	:	:	:
CV1-99986	OTHR136947	65.0	5	QAQCCV	TPH
OTHR348962	OTHR147989	74.85	6	UNK	TPH
OTHR389012	OTHR384702	85.03	7	UNK	TPH
:	:	:	:	:	:
CV2-99986	OTHR427034	65.0	10	QAQCCV	TPH

Weighing Samples

See [Quality Assurance/Quality Control](#) for sample amounts and explanation of sample codes.

1. If a weight recording chart is not available on the SRA PC desktop, prepare a weight recording chart with the following headers (see table above):
 - **Text ID:** copy new text ID from Cahn software window after uploading the mass
 - **Mass:** sample amount weighed into crucible (mg)
 - **Container number:** same as autosampler tray number the sample will be placed in
 - **LIMS code:** Objective - Mass (part of sample): QA/QC - QAQC
 - **SRA code:**
 - **BLK:** calibration blank
 - **STD:** calibration standard
 - **TPH:** unknown sample, QA/QC_blank, QAQC_CV
2. Wipe sample filler, spatula, and forceps with methanol.
3. Log into the balance system for Cahn electrobalance using LIMS user ID.
4. Click **Test Options**, enter a value from 150 to 200, then click **Save/Exit**.
5. Place weighing paper on both balance pans, close the door, and click **Tare** and **Start** on the balance software main screen.
6. Once the measurement is completed and the value is acceptable, click **Get Mass** at the bottom of the *Dual Balance Plot* area.
7. Place sample on the weighing paper in the left pan and click **Weigh** and **Start** on the screen.
8. Once the measurement is completed and value is acceptable (S1 not equal to 0), click **Get Mass**.
9. Place weighed sample material in a crucible using sample filter.
10. Select **Mass (part of sample)** from the *Objective* drop-down list, enter a part of the text ID in the box below *Objective*, and click **Search**.
11. Highlight the appropriate sample from the search list and click **Assign**.
12. Click **Save** at the bottom left of the screen to save mass with a measurement code to LIMS.
13. Write text ID for child sample, mass, container number, and codes in weight chart.

Sample Analysis

Sample analysis workflow is as follows:

- Prepare the instrument (see [Preparing the SRA Instrument](#)).
- Set up software for sequence acquisition (see [Setting up the Software](#)).
- Acquire samples (see [Running Samples](#)).

Preparing the SRA Instrument

The SRA goes through an intense warm-up for 3 hr before operation. Perform the following steps to prepare for sample acquisition (Note: the onboard technician will warm up the instrument):

1. Open H₂, He, O₂, and air gas lines. **Note:** Verify gas gauge pressures using the gas flow meter (see the *SR Analyzer Advanced User Guide*).
2. Turn on the SR Analyzer power.
3. Turn on the PC. **Note:** If more than SRA, computer, and monitor are connected to the UPS, wait 10 min after turning on the SR Analyzer before turning on the PC.
4. Double-click the **TStationAcq.exe** shortcut icon on the desktop to open the software *Main Menu* ([Figure 5](#)).
5. Click **Preview** to confirm oven and FID temperatures. Values will be <300°C. If after 10–15 min oven and FID temperatures have not achieved increased, proceed to Steps 6 and 7.
6. Click **Configuration** and select the **Temperatures** tab.
7. Set desired temperature and click **Send Temperatures Immediately**. **Note:** Except for this action, do not change any values on any tabs in the *Configuration* screen.

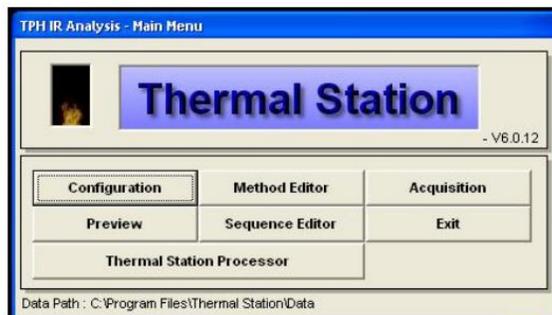


Figure 5. SRA Main Menu Screen.

Setting up the Software

Prepare the software for data acquisition as follows:

- Create a data folder
- Edit the method (if needed)
- Edit the sequence table

Creating a New Folder

Data (CSV and ROW files) are saved into the expedition-specific data folder with the PAS file (sequence record) and PAR file (method) with respect to each sequence (batch).

- Open the Data folder at C:\Program Files\Thermal Station\Data.
- Create a new folder named EXPxxx where xxx is the expedition number (or xxxx in the rare cases where the expedition has a letter designation with it)

Editing the Method

The method does not need to be edited for regular onboard measurements (i.e., safety monitoring) except for the standard information. The onboard laboratory specialist will edit the fields in the **Standard** tab if the standard material changes. In that case, one blank, one standard, and one known sample (house standard) must be measured to confirm calibration (see [Quality Assurance/Quality Control](#)).

The default method is **toc_580** and contains the following tabs:

- Acquisition tab ([Figure 6](#))
- Temperatures tab ([Figure 7](#))
- Standard tab ([Figure 8](#))

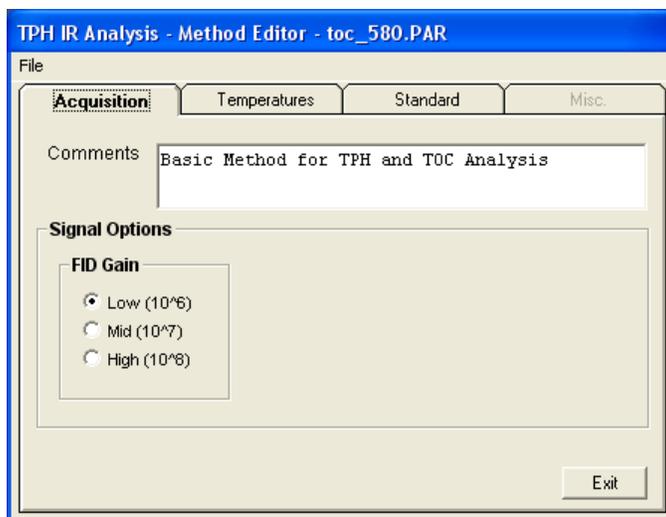


Figure 6. SRA > Method Editor > Acquisition Tab.

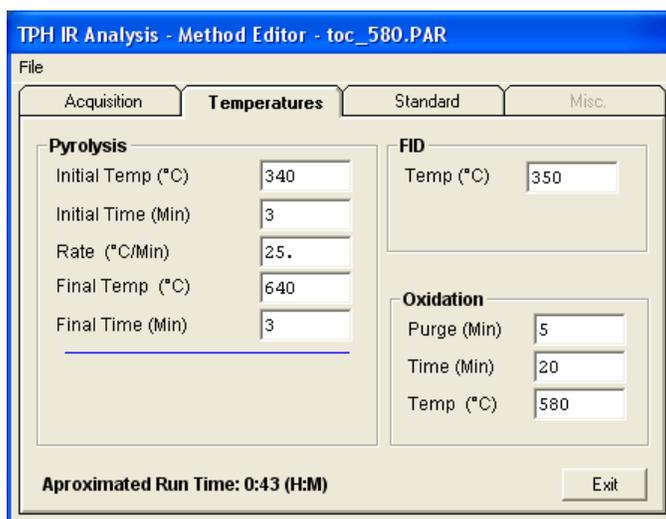


Figure 7. SRA > Method Editor > Temperatures Tab.

TPH IR Analysis - Method Editor - toc_580.PAR

File

Acquisition Temperatures **Standard** Misc.

Calibration Standard Data

Name: 99986

tTemp °C (True Tmax): 457.0 vOCC(S3): 0.39

pTPH mg/grams (S2): 8.41 S4: 23.99

Calibration Temperature Offset: -2.354462°

Calibration FID Response: 1.096987E+08

Calibration FID Baseline: 2.80mV

Calibration IR S3: 3.80E+7 S4: 5.36E+8

Calibration IR Baseline: CO2: 25.84mV CO: 952.07mV

Exit

Figure 8. SRA > Method Editor > Standard Tab.

Editing the Sequence Table

A sequence table represents an analytical batch (see [Quality Assurance/Quality Control](#) for information about batches and calibration). The sequence file is an archive file that is updated with respect to each run. After each batch, the sequence table is saved into the expedition-specific data folder. A typical sequence table contains the following (see [Figure 9](#)):

- *Data File* name (one for each QA/QC and unknown sample to be run). Examples:
 - Calibration blank: OTHR468061
 - Calibration standard: PWDR5
 - Calibration verification standard: PWDR468051
 - Unknown samples: textID = LIMS text ID
- *Sample ID*: must be identical to the Text ID or the LIMS uploader will reject the file
- *Method*: **toc_580** (original method is archived in folder **C:\Program Files\Thermal Station**)
- *C#*: container number (must match autosampler place number, as recorded in the weight recording chart)
- *Sample Weight*: from weight recording chart (mg)
- *Acq Type*: acquisition type
 - BLK = Calibration blank
 - STD = Calibration standard
 - TPH = Unknown samples or QA/QC control samples

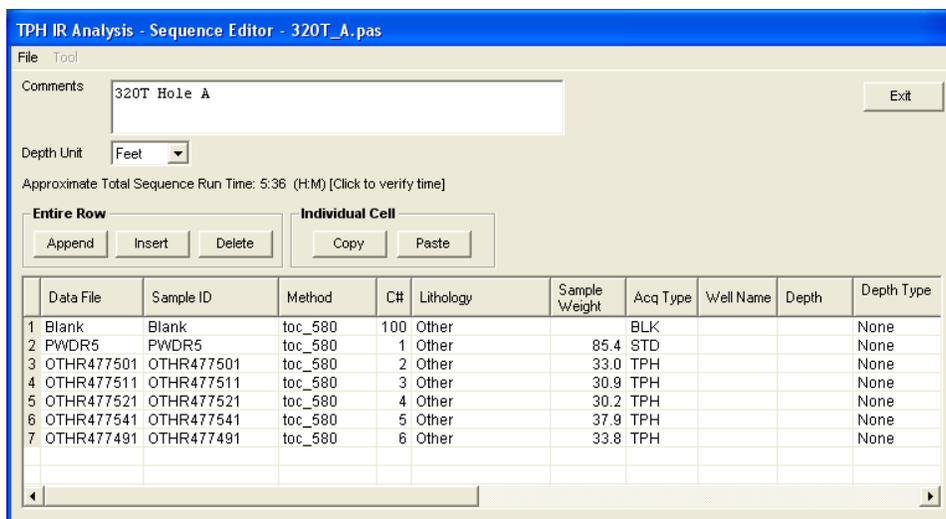


Figure 9. SRA > Sequence Editor > Sequence Table.

Edit the sequence table as follows:

1. Click **Sequence Editor** on the *Main Menu* (Figure 5).
2. Fill in the *Data File*, *Sample ID*, *Method*, *C#*, *Sample Weight*, and *Acq Type* fields using the weight recording chart as a reference.
3. Make sure all information is correctly entered in the sequence table.
4. Click **Exit** at the top right of the *Sequence Editor* screen (Figure 9).
5. To save the edited sequence table, click **Yes**.
6. Save the sequence into folder *C:\Program Files\Thermal Station* (same level as the data folder), as **EXPxxx.PAS**.

Running Samples

To analyze samples, fill in the *Acquisition Setup* screen and confirm sample information on the *Analysis* screen.

1. Select *Main Menu > Acquisition* to open the *Acquisition Setup* screen (Figure 10). Fill in the fields:
 - *Operator*: operator's last name. This name is the key to access LIMS.
 - *Sample Selection*: select the samples to be run from the list shown on the screen.
2. Specify the data folder:
 - Select parent folder **EXPxxx** from the explorer window on the screen.
 - Enter subfolder name **EXPxxx_sequence number** (e.g., **EXP777_1**, **EXP777_2**) in *Data Folder* field.
3. Click **Next** to open the *Analysis* screen (Figure 11).
4. Click **Info** at the bottom right to open detail information and confirm the information for the first sample.
5. Click **Start Sequence** above the sample window to start the run. The software will ask for confirmation of SRA function after starting the first measurement (e.g., autosampler arm position, turn on the FID, etc.).

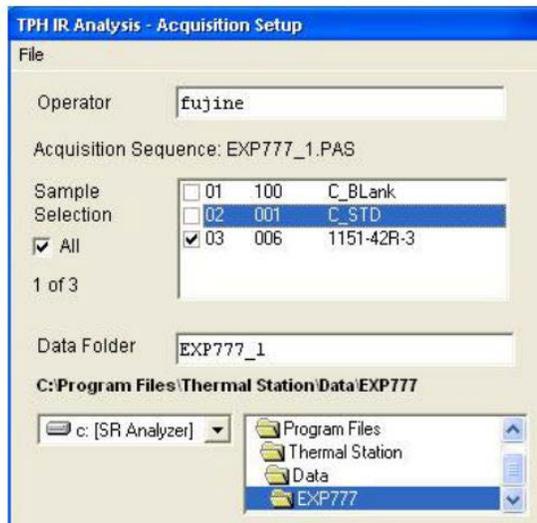


Figure 10. SRA > Acquisition.

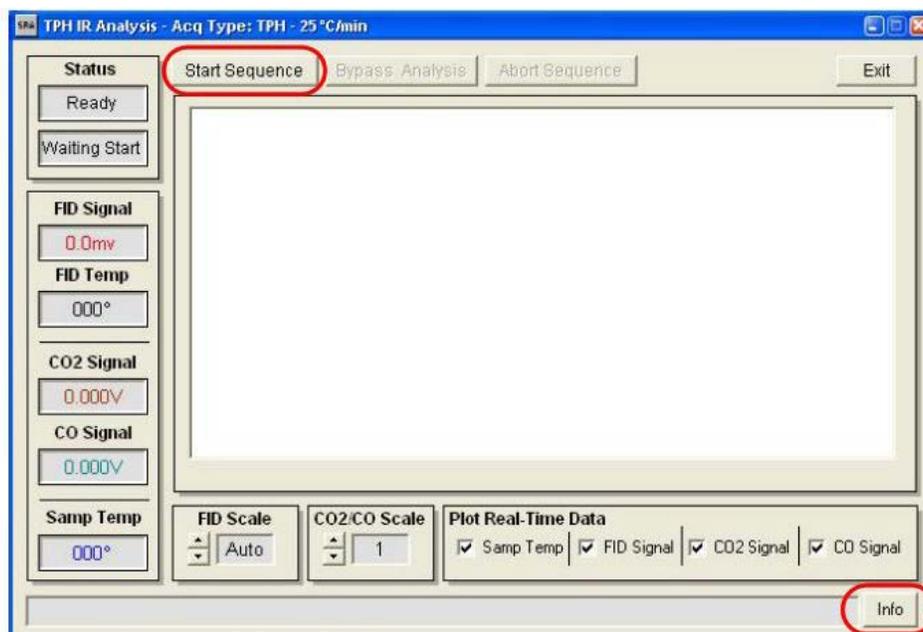


Figure 11. Analysis Screen.

Quality Assurance/Quality Control

Analytical Batch (Sequence)

An analytical batch is referred to as a sequence in this User Guide. Each sequence contains the following samples:

- Calibration blank (CB)
- Calibration standard (CS)
- QA/QC standard (CV)
- QA/QC blank
- Unknown sample(s) (TPH)

Calibration Blank

- The CB blank contains no material
- One CB is included at the beginning of a sequence; mass = 0

Calibration Standard

- Calibration standard is ~80 mg of CS material
- One CS is included in each sequence of 50 samples; more samples require additional calibration
- For smaller batches, the instrument is calibrated once per day

QA/QC Standard

Calibration verification (CV) is conducted for each batch of 10 samples, one of the following:

- CS (60 mg)
- COSS (80 mg)
- Standard 999986 (60 mg); results:
 - S1 = 0.16 mg HC/g
 - S2 = 8.41 mg HC/g
 - S3 = 0.39 mg CO₂/g
 - S4 = 23.99 mg C/g
 - Tmax = 418°C
 - TOC = 3.11 wt%

QA/QC Blank

A QA/QC blank can be measured in either of the following ways:

- Measure an empty used crucible to check background (mass = 1).
- Measure an empty crucible as an unknown (TPH).

Unknown Sample

- 50–70 mg powdered sample material
- Maximum sample = 200 mg

Precision

Precision of analysis is determined by measuring unknown samples in duplicate or triplicate and determining the standard deviation of the replicate samples.

Accuracy

Accuracy is determined by running a calibration verification (CV) with every batch or every 10 samples.

LIMS Integration

Results are stored in the LIMS database associated with an analysis code and an analysis component. Analysis codes and their components, definitions, and units are listed below.

Analysis	Component	Definition	Unit
SRANL	HI	Hydrogen index ($S2 \times 100/TOC$)	mg HC/g TOC
	OI	Oxygen index ($S3 \times 100/TOC$)	mg CO ₂ /g TOC
	PC	Pyrolysis carbon ($0.83 \times [S1 + S2]/10$)	mg HC/g rock
	PI	Production index ($[S1/(S1 + S2)] \times 100$)	—
	S1	HC vaporize < 330°C (free oil)	mg HC/g rock

S2	HC vaporize > 330°C (kerogen)	mg HC/g rock
S3	Carbon dioxide evolved	mg CO ₂ /g rock
S4	Residual carbon	mg HC/g rock
mass	Sample mass	Mg
pdf_filename	SRA PDF filename	—
pdf_asman_id	SRA PDF file ASMAN ID	—
tmax	Maximum S2 (peak) temperature	°C
toc	Total organic carbon	wt%

Creating a PDF File

SRA results are printed to a PDF file, which, along with the corresponding CSV file, are uploaded into the LIMS.

1. Double-click the **TStationProcessor** shortcut icon to open the *Processor* screen (**Figure 12**).
2. Select **File > Open Raw File** to open data.
3. Select the data file to be reviewed and select **File > Print** to create the PDF file. **Note:** The PDF file must be uploaded to LIMS with the CSV file.
4. The file name should be same as the CVS file. Save the PDF file in the same folder as the CSV file.

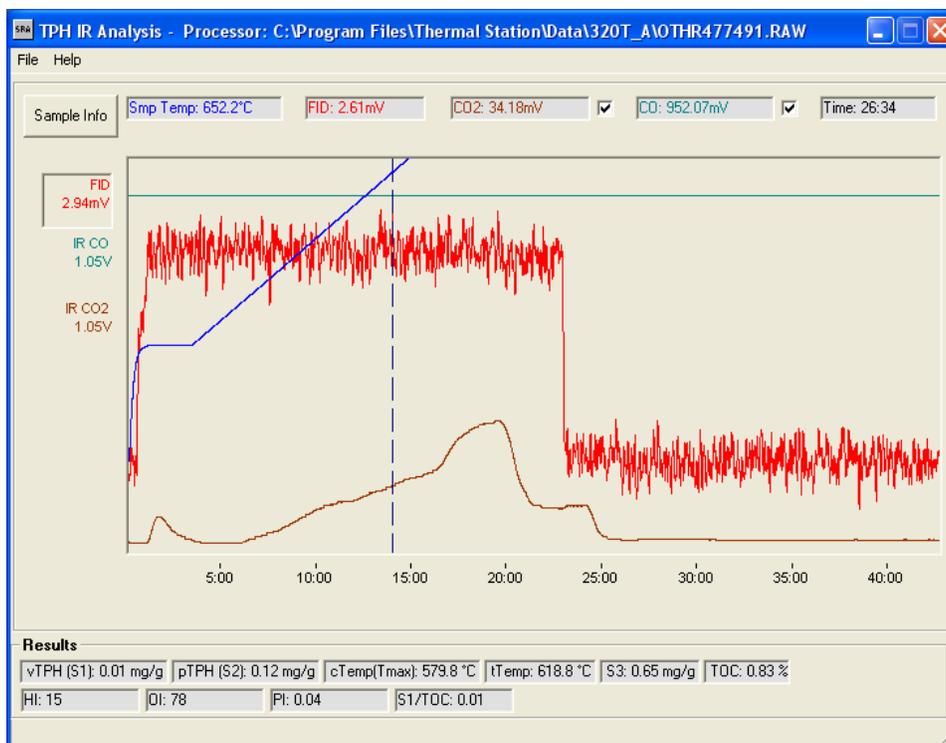


Figure 12. Processor Screen.

Uploading Data to LIMS

The created PDF file along with the corresponding CSV file are uploaded to LIMS.

1. Click **SRAnalyzer Loader** shortcut icon to open the *SR Loader* screen (**Figure 13**).
2. Open CSV and PDF files to be uploaded to LIMS.

3. Confirm *Text_id* and *Operator* name. Edit these fields if needed.
4. Click Calculate to calculate values for *PI*, *PC*, *OI*, and *HI*. Calculated values are shown on the right side of the screen (**Figure 14**).
5. Click **Load** to upload data to LIMS.

The screenshot shows the SR Loader application window. At the top, there are two buttons: "Open CSV" and "Open PDF". Below them are two text input fields labeled "csv filename" and "pdf filename". The main area is titled "Sample Information" and is divided into two columns. The left column, "Fields parsed from file", contains input fields for "Text_id", "mass", "S1", "S2", "S3", "tmax", "loc", and "Operator". The right column, "Fields calculated from leftside", contains input fields for "PI", "PC", "OI", and "HI", along with a checkbox labeled "Is DV?". A "Calculate =>" button is positioned between the two columns. At the bottom right, there are "Load" and "Cancel" buttons.

Figure 13. Loader Screen.

The screenshot shows the SR Loader application window after calculation. The "Open CSV" button is now disabled and shows the file path "E:\Data Analysis\TS112097\TS112907_2\99986_R.CSV". The "Open PDF" button is also disabled and shows the file path "E:\Data Analysis\TS112097\TS112907_2\Thermal Station Processor.pdf". The "Text_id" field contains the value "95310". The "mass" field contains "54.94". The "S1" field contains "0.13". The "S2" field contains "0.44". The "S3" field contains ".25". The "tmax" field contains "419.1772". The "loc" field contains "3.08". The "Operator" field contains "Njine". The "PI" field contains "0.015169194865811". The "PC" field contains "0.71131". The "OI" field contains "0.11680311680312". The "HI" field contains "274.025974025974". The "Is DV?" checkbox is unchecked. The "Calculate =>" button is now disabled. The "Load" and "Cancel" buttons are still present at the bottom right.

Figure 14. Loader Screen with Calculated Values.

Health, Safety, & Environment

Safety

All laboratory specialists must complete required safety training before operating the SRA instrument.

Compressed Gases

- Always wear safety glasses when handling and using compressed gases. Read the MSDS information for the gases used in this procedure.

- Hydrogen gas (CAS 1333-74-0) is highly flammable, explosive limits in air = 4%–74%. Be careful with ignition sources and oxidizers.
- Helium gas (CAS 7440-59-7) is inert but may cause suffocation by displacing oxygen in the air during a release.
- Check for leaks in compressed gas lines.
- Use only wrenches approved for use on compressed gas tanks and lines.
- Ground all equipment and lines associated with hydrogen usage.

High Temperatures

- High oven and detector temperatures (325°–600°C) are reached during operation. Use proper heat protective equipment when operating the instrument.
- Make sure the FID cover is always installed during operation to protect from burns.

Instrument Safety Features

- The instrument will sound an audible alarm if a gas cuts off. Check gas flow and tank pressure if the alarm sounds.

Pollution Prevention

- Trace amounts of pyrolysis products are consumed by the flame ionization detector.
- Helium gas has no adverse ecological effects. It does not contain Class I or Class II ozone-depleting chemicals. Helium is not listed as a marine pollutant by DOT (49 CFR 171).

Waste Management

- This procedure consumes the sample during pyrolysis, so no waste is generated.
 - Sample crucibles are reused.
 - Unused quantities of compressed gases are stored in labeled cylinders with protection cap in place until return to manufacturer.
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