Petrophysics in Gas Shales

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ABSTRACT

A method is described for reservoir characterization in fine-grained and thinly bedded shales based on a probabilistic clustering procedure (PCP) of well logs followed by a forward modeling procedure that results in the calculation of profiles for porosity, water saturation (Sw), and permeability. The credibility of results relies on calibration using porosity, permeability, and mineralogy analyses of core samples. Complementary analysis using a nuclear spectroscopy log, if available, can add confidence to the results.

Kerogen needs to be included during the forward modeling because it is a matrix component of the bulk rock and the matrix grain density (GD) can be significantly affected by kerogen. Kerogen profiles can be estimated if kerogen core analyses are included in the PCP. In addition, a total organic carbon (TOC) profile, which is needed to determine the amount of adsorbed gas, can be estimated based on core analyses of TOC. The relationships between TOC and kerogen, including a discussion of Rock-Eval pyrolysis, are outlined.

The estimation of free gas gross pay in gas shales is fraught with difficulty because of the vagaries of estimating porosity and Sw. Although not realistic in terms of gross storage capacity, the use of the combination of total porosity (TPOR) and total water saturation (Swt) gives the same pay as the combination of effective porosity (EPOR) and effective water saturation (Swe). However, the combination of EPOR and Swt is ill-construed and results in underestimation of gross pay.

The estimation of adsorbed gas in gas shales relies on a methodology and equations adopted from the coalbed methane industry. The workflow is easily implemented, but the credibility of results hinges on the assumption that the adopted methodology and equations are valid for gas shales, and on having sufficient and proper laboratory-derived gas adsorption isotherm measurements to represent the TOC heterogeneity of the reservoir.

An example is given using analysis of a cored well from the Upper Jurassic Haynesville Shale of northwestern Louisiana and northeastern Texas. The
This chapter discusses petrophysics related to the estimation of porosity, water saturation (Sw), permeability, and pay in gas shales. Included is an overview of concepts regarding total organic carbon (TOC), kerogen, Rock-Eval pyrolysis, adsorbed gas, and adsorption isotherms. These parameters generally are not of concern in conventional reservoirs. The primary purpose of this chapter is to introduce a workflow for petrophysical analysis that involves a forward-modeling procedure that can be used in both unconventional shale-gas reservoirs and conventional reservoirs.

We use the word shale to mean any sedimentary rock that has a large component of clay- and silt-size argillaceous particles. Many gas shales have been recognized to be composed mostly of silt-size grains. For instance, the Barnett Shale is more accurately described to be a siliceous siltstone (R. G. Loucks, 2008, personal communication). Although a better term is probably mudrock for many of these gas-containing rocks, we use shale in this chapter for historical reasons.

A list of mnemonic commonly used in this chapter is provided in Appendix H.

Petrology

Gas shales are typically a mixture of detrital, biogenic, and authigenic or diagenetic material. The petrology and mineralogy of gas shales, particularly the Barnett Shale, have been discussed in several articles (Hickey and Henk, 2007; Loucks and Ruppel, 2007).

The detrital nonbiogenic material is commonly composed mostly of quartz, feldspar, and clay minerals. The clay minerals reported are typically illite, chlorite, mixed-layer illite/smectite (I/S), and sometimes kaolinite. The I/S commonly has a low percentage of expandable (smectitic) layers, generally less than approximately 20% (Miller, 2009).

The biogenic material present in most gas shales typically consists of siliceous and calcareous pelagic microorganisms that have been recrystallized during burial and diagenesis. The original mineralogy of the siliceous biogenic component is generally thought to have been opal A (hydrated silica). However, the diagenetic conversion of opal A to cristobalite to quartz, which has been thoroughly documented, for instance, in the Miocene Monterey Formation (Isaacs, 1983; Graham and Williams, 1985), to date has not been documented for any of the diagenetic quartz in any of the Paleozoic gas shales studied.

Phosphatic materials, both crystalline and amorphous, are also found in some gas shales (Hickey and Henk, 2007). For example, the Barnett Shale contains locally abundant beds (in core scale) and microlaminae (in thin-section scale) that are rich in phosphatic material. Beds with visible phosphatic material are sometimes correlated with very high (>250 API) well-log gamma-ray (GR) signal. In thin-section and scanning electron microscope (SEM) study, the phosphatic-rich zones tend to have abundant fecal material rich in fluoroapatite (Slatt et al., 2012).

The presence of amorphous phosphatic material would present a problem in modeling bulk matrix because it would be difficult to impossible to quantify the amounts present via x-ray diffraction (XRD) or other mineralogy detection means. Chemical analysis accompanied by appropriate partitioning of phosphorus into mineral and amorphous phases would be required.

Two observations are of practical importance concerning the phosphate beds. One is that their presence renders nigh impossible the attempts (commonly done in conventional reservoirs) to relate the GR log signal to clay content (viz., Vshale). This is because the high GR signal in the phosphate beds is caused apparently by U or Th, or both, associated with the phosphatic material and not by the K in illicitic clays. The other observation is that the phosphate beds have been identified (in core in the Barnett Shale) as a recognizable component of some lithofacies stacking patterns that are mappable via well logs (Singh, 2008; Slatt et al., 2012).

Nonbiogenic authigenic (formed at shallow burial depths) and diagenetic (formed or recrystallized at relatively deep burial depths) minerals include dolomite, ankerite, siderite, and pyrite. The first three are carbonates, and the last three are rich in iron. Ankerite is iron-rich dolomite and generally cannot be distinguished from dolomite during routine thin-section study or during routine XRD analysis. Because the iron-rich minerals significantly affect the matrix grain
density (GD) and the photoelectric (PE) log response, they should be characterized and modeled as accurately as possible.

Another matrix component is kerogen. Because kerogen is a solid, it should be included in any attempt to model the matrix components when modeling the bulk composition of a gas shale. The manner in which we do this is discussed below.

Quantitative assessment of relative amounts of nonbiogenic (detrital) versus biogenic sediment components relies on laborious and sometimes difficult examination via microscopic and SEM study.

The XRD cannot discriminate between recrystallized biogenic silica (now quartz) and detrital quartz. A common method for representing the XRD-determined mineralogy of siliceous shales is via ternary diagrams (Loucks and Ruppel, 2007) using these as end members: total clay minerals, total carbonate minerals (calcite + dolomite + ankerite + siderite), and remaining components (quartz, feldspar, pyrite, and phosphate). These diagrams are useful for illustrating the gradational nature of the mineralogy of lithofacies in a vertical interval but will mask desired information concerning sediment origin unless the XRD results are accompanied by a detailed thin-section study.

### Petrophysics

#### Porosity

Such a seemingly simple concept as porosity is difficult to define and quantify in fine-grained rocks. In gas shales, unlike in many conventional reservoirs, the small grains are not restricted to the clay minerals; instead, even the siliceous and calcareous components are commonly on the same size range as the clay minerals. The small grain size results in small pores and narrow pore throats, and this causes difficulties in laboratory measurements of interparticle porosity and in modeling pore-size and pore-throat distributions. The situation is further complicated by reports that substantial gas-shale porosity exists as holes in organic material that have developed during thermal maturation (Ruppel and Loucks, 2008; Loucks et al., 2009).

The physiochemical reaction of clay minerals with pore waters results in a certain fraction of the water in the pores being bound to the clay surfaces. Because this fraction of the pore water is not part of the free water and also presumably cannot contain hydrocarbons (HCs), it is important to quantify the amount of this bound water. Quantification using well-log analysis requires a good understanding of the bulk composition of the rock and some method of modeling this composition.

#### Water Saturation

Total Sw (Swt) is the fraction of porosity that is occupied by water of all types (e.g., bound plus free). The rest of the porosity is occupied by HC. In any bulk rock model, each porosity type needs to be explicitly defined and the Sw quantified. One way of doing this is discussed later in this chapter.

#### Permeability

Most gas-shale wells require hydraulic fracturing (fracing) to establish gas production because the intrinsic permeabilities are generally only in the range $10^{-4}$ to $10^{-8}$ md. Although fracing opens up channels to the wellbore, the intrinsic matrix permeability is important for permitting gas to move into the frac channels. So, variations in the magnitude of the matrix permeability are important to decipher.

In many gas shales, it is impossible to retrieve standard core plugs from most lithologies because of the tendency for the rocks to part along bedding surfaces of the finely laminated beds (Miller, 2009). Even if retrieval of standard core plugs were possible, the economics of conducting permeability flow tests over the very long times necessary for the fluids to move through the rocks would mean that standard plug analysis of every foot of core would rarely be done.

Because of convenience and cost, permeability estimates are commonly made on crushed samples. Any analyst needs to be aware of the procedures, credibility, and limitations of such data (Bustin et al., 2008). If possible, any such measurements should be calibrated against normal flow permeability measurements.

#### Pay

We divide pay for gas shales into two types. Gross pay is the amount of in-situ HC present in the rock. Net pay is the amount of in-situ HC that might be recoverable during a frac-induced extraction program. Because of the vagaries (and our general ignorance) associated with what happens during fracing (i.e., fracture geometry, fracture extent, reservoir pressure, etc.), we do not address net pay in this chapter.

Gross gas pay (henceforth, pay) is generally divided into free gas pay and adsorbed gas pay. Each of
these two volumes is estimated differently, with each having associated challenges.

The main problems with estimating free gas pay involve knowing

1) in which porosity type the gas is located, how the amount of each porosity type can be determined, and how much gas is in each type;
2) an appropriate Sw definition and how that saturation can be determined; and
3) assuming that pay flags are to be used, which parameters are to be used as flags?

For instance, possibilities are some combination of total porosity (TPOR), effective porosity (EPOR), total water saturation (Swt), effective water saturation (Swe), permeability (K), and bulk volume water (BVW).

Estimation of adsorbed gas is typically done by

1) estimating the amount of kerogen in the rock and then
2) estimating the amount of gas that would be adsorbed to the kerogen at reservoir temperature and pressure.

The amount of kerogen in the rock is estimated by either converting bulk rock TOC measurements to kerogen content (using conversion factors that consider the kerogen type and maturity) or from Rock-Eval analyses.

Estimation of the amount of gas adsorbed to the kerogen at reservoir conditions is commonly done from gas adsorption isotherm studies on core samples of known kerogen content. The studies are done at reservoir temperature over a range of pressure to generate an adsorption isotherm, which is a graph of gas adsorbed versus pressure. Then, although perhaps not a good assumption (Bustin et al., 2009), the adsorbed gas capacity obtained from the isotherm is assumed to represent the amount of gas adsorbed to the kerogen in the reservoir.

Although it is common practice to relate TOC, kerogen content, and kerogen adsorption capacity (of gas) via empirical equations developed for the coalbed methane industry (R. Lewis, 2004, personal communication), to our knowledge, the validity of applying these equations (with their associated constants) directly to gas shales has not been demonstrated.

Once the gas adsorption capacity (i.e., the adsorbed gas component of gross pay) has been estimated, the adsorbed gas net pay component is estimated by assuming that desorption would occur, following the adsorption isotherm, as reservoir pressure declines during production of free gas.

In summary, estimation of gross pay is challenging for shale-gas formations, and to handle high levels of uncertainty, probabilistic approaches could be useful. The estimation of net productive pay by petrophysical means alone is difficult because of the dependence on making assumptions about the results of the engineering (hydraulic fracturing/stimulation) program. Because of this, a concerted effort to synthesize the geology-petrophysical model with the engineering-reservoir model (via history matching) is extremely important.

METHODS

Overview

The evaluation of gas shales using statistical and probabilistic or log overlay techniques has been proposed and used in the past (Passe et al., 1990; Spears and Jackson, 2009). The method described herein relies upon forward modeling of core-calibrated well-log responses to estimate key formation properties useful in the evaluation of producing gas-shale formations.

Three key aspects to the workflow are the generation of a variable GD profile, a variable clay content profile, and a variable matrix surface area profile.

- The GD profile is used in a density-porosity (DPHI) equation to compute TPOR.
- The variable clay content profile is used to compute a variable cation exchange capacity (CEC) that is used to compute a variable clay conductivity term (Qv), which in turn is used in a dual-water (DW) model (Clavier et al., 1977) to compute the Sw.
- The variable matrix surface area (SA) profile is used, along with porosity and GD, to estimate the permeability (Herron et al., 1998).

The above is done within a forward modeling routine that is part of the software Geologic Analysis via Maximum Likelihood System (GAMLS®), manufactured by Eric Geoscience, Inc. The forward modeling generates synthetic profiles for GD, bulk density, neutron response, and photoelectric response. The goal for the latter three is to adjust inputs so that the synthetic curves mimic the downhole well-log density (RHOB), neutron (NPHI), and photoelectric factor (PEF) curves. Once a suitable match is made for these
curves (particularly, the NPHI curve), plus once cer-
tain other balance criteria are met (see Balance [For-
ward Model Quality Control] section), then the
resulting profiles for GD, Qv, and SA are used in the
computation of TPOR, Sw, and permeability.

The forward modeling routine can be used in any
type of conventional reservoir, but it is particularly
useful in unconventional gas shales because of the
nature of these rocks and because of how the forward
modeling works. Specifically, (1) gas shales are gen-
erally very finely bedded with a mineralogy and a
reservoir quality that generally change gradually, not
abruptly, with depth; and (2) the forward modeling
assigns distinct properties to each sample depth based
on the probabilistic assignment of each sample to one
or more of several end-member rock types.

Classification of Rock Types

A probabilistic clustering and prediction (PCP)
method is used to delineate rocks with a similar char-
acter and to estimate values for missing (null) data.
The clustering engine is a routine within the software
GAMLS. Previous studies that have used this cluster-
ing engine include Gonzalez et al. (2008) and Slatt et al.
(2008).

Clustering

The clustering procedure groups all (digitized) sam-
ples into one or more end-member electrofacies. These
electrofacies are considered to be analogous to litho-
facies or rock types. The mathematical term used for
these clusters of data is modes. The clustering is
done probabilistically so that a given sample can
belong to more than one mode. To set up a clustering
run, the wells, depth ranges, clustering variables, num-
ber of modes desired, and an initialization method are
selected. Initialization determines the initial probabil-
ity assignments for each sample.

A clustering run is an iterative procedure that
reassigns the initial probability distributions to sat-
ify an imposed model. The imposed model forces a
reassignment of the initial probabilities such that the
frequency distribution of each clustering variable is
divided into \( m \) pseudo-Gaussian distributions where
\( m \) = number of modes. For example, if 10 modes
(lithofacies) are requested, the total GR frequency
distribution for all samples, for all wells used, will be
divided into 10 pseudo-Gaussian distributions each
representing a lithofacies. If four clustering variables
are used (e.g., RHOB, NPHI, GR, PEF), the resulting 10
modes can be visualized as occupying a four-
dimensional space in which some samples will be
assigned to only one mode, but many will be partially
assigned to two or more modes.

Samples can be envisioned to be mixtures of dis-
crete end-member lithofacies, and the clustering pro-
cess generates a realization that assigns the probability
that each sample belongs to each of the end-member
lithofacies. This classification procedure is particularly
suitable for gas shales that have a mineralogy and a
texture that typically change gradually with a higher
frequency than can be readily interpreted by the usual
processing of well logs.

Prediction

The petrophysical work flow includes a step that
estimates values for missing or nulled spurious data.
This prediction part of PCP occurs automatically dur-
ing clustering. Values are estimated from the covari-
ance of the modes in v-space where “v” is the number
or variables used in the clustering analysis.

Clustering variables can be any type of data, not
just well logs. For example, a complete profile for TOC
can be generated if sufficient TOC core analyses have
been made and if TOC is included as a clustering
variable.

Lithology Estimation

The modes defined by clustering are automatically
assigned to a generic rock type using a routine that
uses the mean GR signal for clastic rock types (sand-
stone, siltstone, and shale) and apparent GD for car-
bonate rock types (limestone and dolostone). The
logic for making these assignments is user driven,
and the assignments can be overridden (Eslinger,
2007).

In gas shales, because the most abundant rock type
is generally shale, many of the modes defined by
clustering will be a shale, but there likely will be
several shale modes each representing a different
modeled end-member shale. For instance, if a clus-
tering run is made in which 10 modes have been
requested, the lithology of the resulting modes might
be interpreted to be three siltstones, four shales, two
limestones, and one dolostone. Each of these 10 end
members is defined in v-space by a mean and stan-
dard deviation not only for each clustering variable
but also for all other variables in the imported Log
ASCII Standard (LAS) file. The mean and standard
deviceation of these variables are computed for all wells
included in the clustering run.

The results of a clustering run are readily visualized
in a depth plot where the probability assignments are
plotted on the horizontal axis (see track 2 in a subsequent figure). These results generate a geologic framework for stratigraphic interpretation, and they are also essential for the forward modeling used to generate porosity, Sw, and permeability profiles.

**Forward Modeling**

Forward modeling involves modeling of several parameters and is most reliable when calibrated with data from cored wells. The general procedure is for both cored and noncored wells to be included in a multiwell clustering run. Once a credible forward model is developed for a cored well, the model then can be applied to the noncored wells that were included in the clustering run.

**Porosity**

The bulk rock is modeled using the components shown in Figure 1 (revised from Hill et al., 1979). The matrix components include minerals plus kerogen. The H atoms of OH in clay minerals are detected by neutron logs, but they are not part of the TPOR. Instead, this structural water (of petrophysics literature) is part of the matrix and is not released from the crystalline structure below dehydroxylation temperatures of approximately 550 to 600°C.

The fluid components include water and HCs partitioned into different porosity types. The porosity types are classified as follows.

\[
TPOR = \text{total porosity} = \text{BPOR} + \text{IPOR} + \text{FPOR}
\]

where

- \( \text{BPOR} = \text{bound water porosity} \)
- \( \text{IPOR} = \text{irreducible fluids porosity} \)
- \( \text{FPOR} = \text{free porosity} \)

\[
\text{EPOR} = \text{effective porosity} = \text{IPOR} + \text{FPOR}
\]

\[
\text{IPOR} = \text{irreducible porosity water} + \text{irreducible porosity hydrocarbon} = \text{IPORW} + \text{IPORH}
\]

\[
\text{FPOR} = \text{free porosity water} + \text{free porosity hydrocarbon} = \text{FPORW} + \text{FPORH}
\]

Thus,

\[
\text{EPOR} = (\text{IPORW} + \text{IPORH}) + (\text{FPORW} + \text{FPORH})
\]

For rocks devoid of clay minerals (i.e., some conventional reservoirs), BPOR is zero, and IPOR can be estimated using capillary pressure (Pc) tests. In gas

**Figure 1.** Box model used for modeling components of gas shales (revised from Hill et al., 1979). Ill = illite; Chl = chlorite; I/S = illite/smectite; Qtz = quartz; Dol = dolomite; Cal = calcite; Ank = ankerite; Pyr = pyrite; Sid = siderite; Fsp = feldspar; Oh = hydroxyl groups.
shales, BPOR is never zero, and it is likely that at least some of it effectively becomes part of the IPOR that is estimated in high-pressure capillary measurements.

If HCs cannot exist in true capillary IPOR not associated with clay minerals, the fact that Pc measurements might include BPOR does not affect the determination of Sw. However, because most gas shales are sourced within the reservoir, it seems possible that some fraction of IPOR contains in-situ gas. Further work is needed to prove or disprove this notion.

The possibility that some HCs might exist in the IPOR volume is generally ignored in the case of conventional reservoirs that are presumably water wet and HC-charged from an external source rock. In gas shales that are both source and reservoir, this assumption is less reliable, but for practical reasons (viz., having no credible way to know the fraction of IPOR occupied by HCs), the assumption might be that IPOR contains no HC. However, if a nuclear magnetic resonance log is available, FPOR can be estimated. Then, if TPOR-BVW > free porosity (where BVW = total bulk volume water = [TPOR] [Swt]) and free porosity is from the nuclear magnetic resonance log, there must be some HC in the IPOR.

In gas shales, it seems likely that the division between irreducible porosity and free porosity is a continuum instead of a sharp boundary in terms of pore-size and pore-throat distribution. So, the definition of irreducible porosity is not a theoretical one that can be easily tested by laboratory experiments. Instead, it seems that the numerical value of IPOR for a given rock will depend on the laboratory equipment and procedure used to conduct a capillary pressure measurement. Because the very poor reproducibility of Pc measurements of clay-free sandstones has been demonstrated (M. Globe, 2009, personal communication), we would not expect that reproducibility of measurements made on shales would be any better.

Although BPOR can be estimated from a knowledge of the clay mineral content (see below), the determination of IPOR in shales is more problematic. An interpretation of high-pressure mercury Pc measurements in shales suffers from knowing the theoretical maximum pore space (including the percentage of BPOR occupied by water at reservoir conditions) that, after cleaning the sample, might be occupied by mercury at high pressures without distorting the matrix geometry.

An alternative model assumes that BPOR can be occupied by helium during porosity determination and by mercury during Pc measurements and that the rock texture is not disrupted during cleaning or during the Pc test.

Then, assume that the IPOR that is typically interpreted from Pc analyses of shales can be divided into two components:

1) \( \text{IPOR}_B = \text{irreducible fluids porosity that is equal to BPOR} \)

2) \( \text{IPOR}_C = \text{irreducible fluids porosity (not associated with BPOR) that is caused by capillary forces associated with pores and pore throats among very small grains} \)

The BPOR can be computed using TPOR, the bulk rock CEC, the bulk rock GD, and the pore water salinity (cf. Clavier et al., 1977).

By considering \( \text{IPORB} \) to be equivalent to BPOR,

\[
\text{IPOR}_C = \left( \frac{\text{Swir}}{\text{TPOR}} \right) - \text{IPOR}_B
\]

where Swir is irreducible water saturation.

Then, free porosity, the only component of porosity in which free gas is assumed to exist, is

\[
\text{FPOR} = \frac{\text{TPOR} - (\text{BPOR} + \text{IPOR}_C)}{(1 - \text{Swir})/\text{TPOR}}
\]

However, this argument is valid only for native state (prestimulation) conditions. During hydraulic fracturing, some of the gas contained in IPOR is released and becomes part of the free gas.

But even if this model approximates reality, the small number of Pc measurements that would typically be made might not sufficiently describe the rock heterogeneity in a reservoir, and even if it did, a method of relating these results to well logs would be needed to develop a continuous profile showing the relative amounts of BPOR, IPOR, and FPOR.

The approach that we use for estimating IPOR (when a nuclear magnetic resonance log has not been run) is to use the following empirical equation developed for conventional reservoirs (M. Herron, 2000, personal communication).

\[
(\text{BPOR} + \text{IPOR}) = \frac{\text{TPOR}}{\left[ \left( \frac{K^{0.25}}{10 \times \text{TPOR}^{0.5}} \right) + 1.0 \right]}
\]

where \( K \) = permeability (md) estimated using the Herron et al. (1998) method (see Permeability section below). Then, it follows that

\[
\text{IPOR} = (\text{BPOR} + \text{IPOR}) - \text{BPOR}
\]
In the forward modeling procedure, porosity balance refers to the desired constraint that in tight (FPOR = 0) wet rocks, \( \frac{(BPOR + IPOR)}{C^{24}} \approx TPOR \). A porosity balance is computed for each sample, and the mean value is computed for each mode. Within the forward modeling, the empirically determined exponents for K and TPOR can be adjusted to help achieve porosity balance. In addition, an IPOR adjustment factor (IPOR_Ftr) can be implemented to adjust the mean IPOR to obtain a porosity balance for that mode.

**Water Saturation**

A DW model (Clavier et al., 1977) is used for computing Sw. The key aspect of this equation is a clay-conductivity term, Qv, that accounts for the conductivity of clay-bound water (BPOR). The Qv is computed from the CEC and the pore volume. Details are discussed in Appendix B.

Given reliable clay mineral characterization of rocks, the total matrix rock CEC can be estimated via mass balance by assigning CEC values for end-member clay mineral types. Although CEC values vary within a given clay mineral group (smectites, illites, kaolinites, chlorites) with grain or crystal size, and for smectites, with the structure and chemistry, we commonly use average values of analyses of standard samples (see Appendix B). Within the forward modeling procedure, default CEC values (Herron and Matteson, 1993) are included within a log tool response table.

The forward modeling method requires insertion of the weight percentage of each mineral for each mode. The CEC values for each mineral are then used to compute the mean CEC of each mode using

\[
CEC = \text{Sum}(CECi \times Wi)
\]

and then the mean CEC of each sample (digitized depth) is computed using the fractional probability assignments for each sample assigned during the clustering run. The CEC is then divided by the porosity to obtain Qv.

The effect of the clay on electrical conductivity is handled by the Qv term in the DW equation (Clavier et al., 1977). The effect of the clay on reducing TPOR is handled by a computation (part of the DW method) that assigns a volume to the clay-bound water. In the Clavier et al. (1977) method, the volume of the clay itself is not subtracted from TPOR; instead, the volume of the clay-bound water is subtracted.

The forward modeling method does not circumvent the need to obtain representative mineralogy data or CEC data for each of the major rock types. However, it does provide a means to input real or estimated data and then to compute for each sample a unique value of CEC using the probability assignments from the PCP results. It also provides a means to readily change the input parameters and to quickly observe the results on the computed values of EPOR and Sw.

**Permeability**

Permeability is estimated using a method described by Herron et al. (1998). Although their article focuses on siliciclastics, subsequent work (M. Herron, 1993, personal communication) has used the method in carbonates. In practice, we have used the method for conventional siliciclastics and carbonates and for gas shales and find the method useful for each of these rock types.

Herron et al. (1998) developed equations based on measurements (Sen et al., 1990) for porosity, formation factor, specific surface area, matrix density, and permeability that permit estimation of permeability. We use the mineralogic form of the Herron method (Herron et al., 1998), which requires inputs for the sample porosity, mineralogy (in weight percent), GD, and mineral surface area. The method and equations are described in Appendix D.

The determination of the surface area (SA) of a given rock type relies on the presence of reliable mineralogy data and on knowing the SA of each of the minerals present. Because surface areas typically vary with grain size, the forward modeling mineral tool response database permits multiple entries of a given mineral (e.g., quartz) so that surface areas for different grain sizes can be used. The mean mineralogy of a given mode then can be modeled to include, for instance, 23% very fine-grained quartz and 16% silt-size quartz. The mineralogies and the surface areas are inputted for each mode, and the resulting SA for each sample is computed via mass balance using the fractional probability assignments from the PCP clustering run. In practice, the mineralogies and particularly the surface areas are adjusted until the resulting estimated permeability values approximately agree with any laboratory-measured permeability data from the core. This process is analogous to computing the GD or the TPOR of each sample (previously described).
Kerogen

A short definition of kerogen is that it is the solid insoluble (in organic acids) component of the organic material of rocks. Bitumen is the soluble organic component (Hutton et al., 1994).

Because kerogen is a solid, it needs to be included in modeling of the rock matrix, whereas TOC is needed to estimate the amount of adsorbed gas (Appendix E). Because a large part of kerogen is organic carbon, kerogen content is related to TOC, but they are not equivalent. Conversion factors are discussed below and in Appendices E and F.

Total Organic Carbon Versus Kerogen

The TOC measurements are commonly done using pyrolysis of core samples. Samples are acidified then heated in an oxygen atmosphere. Carbon reacts with oxygen to form CO$_2$, which is measured in a detection cell (Bernard et al., 2009). Weight percent CO$_2$ is converted to weight percent C and reported as weight percent TOC in the rock.

The acidification is done to remove soluble carbonates. The Barnard et al. method uses phosphoric acid, but hydrochloric acid can be used (Jarvie, 2009). However, because dolomite, ankerite, and siderite are fairly resistant to acid dissolution at room temperature, higher acid strengths or higher dissolution temperatures than used for the usual calcite dissolution (dilute HCl at room temperature) might be required for dolomite, ankerite, and siderite dissolution. Unless care is taken to completely remove these minerals, TOC analyses might be misleadingly too high in gas shale samples that contain them. A means of correcting TOC analyses that have been made without removing these minerals is outlined in Appendix F.

Kerogen is qualitatively characterized (into type I, type II, type III, etc.; Tissot and Welte, 1984) using special microscopic techniques, but quantification commonly is done using Rock-Eval pyrolysis (Espitalie et al., 1977; Jarvie and Lundell, 2001; Boyer et al., 2006). A rock sample is heated (after acidification) at a controlled rate and gases evolved over four temperature ranges are measured and resolved into four peaks (S$_1$–S$_4$). The S$_2$ peak occurs between temperatures of approximately 300 to 600°C [572 to 1112°F] and is interpreted to be caused by CO$_2$ resulting from interaction of ambient oxygen in the apparatus with organic carbon in the kerogen of the sample. The results are reported as milligrams of HC per gram of rock.

Note that this kerogen quantification (from the S$_2$ peak) gives not the amount of kerogen in the rock, but the HC-generating potential of the remaining kerogen. If the rock is not thermally immature, it will already have generated some gas, and its kerogen-generating potential will have decreased. Thus, the S$_2$ peak decreases with thermal maturity. The amount of original kerogen also decreases with thermal maturity because kerogen is gradually destroyed (cracked) during maturation. Because the amount of kerogen decreases, the amount of TOC in the bulk rock also decreases, but they decrease at different rates. This means that a constant conversion factor does not exist for converting between weight percent kerogen and weight percent TOC. Instead, the kerogen/TOC ratio is a function of thermal maturity (and kerogen type).

In an analogous manner, the ratio of HC (S$_2$ peak) to TOC—which is termed the hydrogen index (HI)—decreases with thermal maturity. The trend of decreasing HI with increasing thermal maturity is caused by the fact that H is preferentially lost relative to C during thermal maturation.

Kerogen Properties

Although kerogen is organic, it is treated as a discrete mineral component during the forward modeling procedure. Kerogen parameters required are GD, CEC, SA, and HI for each matrix component. Modeling of PE response is optional but very useful in some cases.

The density of kerogen is used in the modeling of sample GD. Commonly, a value of 1.2 grams per cubic centimeter (g/cc) is used for the density of kerogen in gas shales (Miller, 2009; Spears and Jackson, 2009), but the density can range between about 0.9 and about 1.4 g/cc and generally increases with increasing thermal maturity (Jarvie, 2009). According to Okiongbo et al. (2005), kerogens at high thermal maturity have densities of about 1.35 g/cc.

The density varies with kerogen type and thermal maturity, but its analytical determination is likely problematic because of the difficulty of isolating it. For instance, a density of approximately 0.9 g/cc was determined for kerogen from the Monterey and Sisquoc formations using a combination of chemical and mechanical methods and after correcting the density of the isolated concentrate for disseminated pyrite remaining in the sample (E. Eslinger, 1987, unpublished data).

Although the CEC and surface area of kerogen are used in the modeling of Sw and permeability, respectively, we know of no data on CEC or surface area of kerogen. With considerable temerity, we have assumed that kerogen has approximately the same surface area as illites and smectites (~85–100 m$^2$/g; Van Olphen and Fripiat, 1979) and assign an insignificant CEC of 1 milliequivalent per 100 grams (1 meq/
100 g), which is much lower than that of smectite (~100 meq/100 g; Van Olphen and Fripiat, 1979).

Neutron response (to neutron logging tools) is quantified by the HI. In petrophysics work, HI, which is not the same as the HI of organic chemistry, is defined as (Eslinger and Pevear, 1988):

\[
\left( \frac{r_i}{m_i} \right) / \left( \frac{r_w}{m_w} \right) = \left( \frac{r_w}{m_w} \right) (11)
\]

where

\[
\rho_i = \text{density of component (~mineral) } i
\]

\[
m_i = \text{weight percent of H in component } i
\]

\[
\rho_w = \text{density of water}
\]

\[
m_w = \text{weight percent of H in water}
\]

So, for kerogen, neutron response HI can be estimated, for instance, as

\[
[1.35 \text{ g/cc}(7\%)] / [1.0 \text{ g/cc}(11\%)] = 0.095/0.09 = 0.85
\]

This uses 1.35 g/cc as a density for kerogen and assumes that the weight percentage of H in kerogen is within the range of that found in the analyses of kerogen from the Barnett Shale (Hill et al., 2007; their table 1; cf. Appendix F).

To model the PE response, either Pe (which is a function of chemistry; units are barns/electron [b/e]) is required or it can be computed from Pe = \(U/\rho_e\) if \(U\) (barns per cc) and the electron density (\(\rho_e\)) are known. According to Lewis et al. (2004), \(U\) ranges from 0.18 to 0.24, and PE is similar to coal (~0.16–0.18; R. Lewis, 2008, personal communication).

**Balance (Forward Model Quality Control)**

Credibility of forward modeling is maintained by several balance arguments. The manual adjustment of inputs in search of a solution for simultaneous and multiple balances during forward modeling can be a challenging and laborious task because of the many interacting variables. Accordingly, a genetic algorithm exists within the forward modeling procedure that permits efficient attainment of user-selected balances via multiple objective functions.

**Mineralogy, Grain Density, and Porosity Balance**

Each PCP mode is assigned a mineralogy weight percentage. The mineralogy is assigned using XRD analyses of samples from the mode, if they exist, or an initial estimate of the mineralogy from log analysis data or general knowledge about the reservoir. The GD for each mode is computed, and then the probability assignments are computed from this and the probability assignments:

\[
1/RHOG = \Sigma(m_i)/(RHO_i)
\]

where

\[
\text{RHOG} = \text{sample GD}
\]

\[
m_i = P_i = \text{probability that the sample is assigned to mode } i
\]

\[
RHO_i = \text{GD of mode } i
\]

The fractional mode probability assignments are treated as fractional masses (~weights) of the matrix system (no porosity included in the system). The equation sets total matrix volume (left side of equation 13) to the sum of the fractional volumes of the total matrix of each mode (right side of equation 13).

The computed grain densities for each sample are compared with the grain densities measured from core plugs. This is done on an individual sample basis. In addition, the mean value of GD for each mode is compared with the mean GD of each mode that is measured on core plugs. These differences serve as another modeling balance that can be checked and improved as needed by adjusting inputs.

The computed mineralogy percentages for each sample are compared with the XRD mineralogies measured on core samples. The comparison of modeled mineralogy with quantitative XRD mineralogy is a necessary quality control step to check the mineral balance of the model. The XRD analyses of core samples should be sufficiently accurate to render the procedure credible.

The computed GDs are then used to compute TPOR for each sample using a DPHI equation with a variable GD and a variable fluid density. This variable fluid density currently uses a constant water density, but it does consider Sw, the densities of gas (and oil), and the amount of invasion and the density of the invaded fluid (Appendix G).

The inputs for mineralogy for each mode are iteratively adjusted until the modeled mineralogy, grain density, and total porosity values agree with the core analysis XRD mineralogy, grain density, and porosity values, respectively. Thus, the modeling is calibrated against core data, and the proximity of the balance for modeled mineralogy, grain density, and porosity is the degree to which they match core mineralogy, core grain density, and core porosity. In addition, as discussed in a previous section, an additional porosity balance strives to ensure that in tight (FPOR = 0) wet rocks, (BPOR + IPOR) ~ TPOR.
Synthetic Logs Versus Wireline Well Logs Balance

Synthetic (modeled) well logs can be generated for RHOB, NPHI, GR, PEF, and interval transit time (DT) using the results of the clustering analysis, known or assigned mineralogy for each rock type, and a tool response database. The overall goal is to match the synthetic logs, as closely as possible, to the downhole measured wireline logs. This is done by adjusting the inputs plausibly and honoring any known data.

Modeled RHOB (M_RHOB) is computed as

\[
\text{matrix mass} + \text{water mass} + \text{oil mass} + \text{gas mass} + \text{filtrate mass} = \\
\left[(\text{RHOG})(1 - \text{TPOR})\right] + \\
\left[\text{TPOR} (\text{Swt}) (\rho_w)(1 - \text{Xmf})\right] + \\
\left[(\text{TPOR})(1 - \text{Swt})(1 - \text{GOF}) (\rho_w)(1 - \text{Xmf})\right] + \\
\left[\text{TPOR} (\text{Swt})(\text{GOF}) (\rho_g)(1 - \text{Xmf})\right] + \\
\left[\text{TPOR} (\rho_t)(\text{Xmf})\right]
\] (14)

where

- \text{Swt} = \text{total water saturation via dual water equation}
- \text{GOF} = \text{gas to oil volumetric fraction}
- \text{Xmf} = \text{invasion factor} = \text{fraction of pore fluids replaced by mud filtrate}
- \rho_w, \rho_o, \rho_g, \text{and } \rho_t \text{ are densities of water, oil, gas, and filtrate, respectively}

Provision is also made for inputs for the densities of water, oil, gas, and filtrate.

The most important curve to model is NPHI. In fact, obtaining a good NPHI balance for each clustering mode is a key to the forward modeling procedure. This is also true for conventional reservoirs, not just gas shales. Because the NPHI tool reads H in the bulk rock, NPHI balance is made by adjusting the porosity and the clay content for each mode. All pores contain H in the form of water and HCs, so the higher the porosity, the higher the NPHI response. In the inorganic matrix, the only minerals with any significant H are the clay minerals. So, the higher the clay mineral content, the higher the NPHI response. Equations used for generating modeled NPHI (M_NPHI) are given in Appendix H.

For a given mode, porosity is adjusted by adjusting the GDs of the minerals assigned to that mode or by adjusting the amount of the different clay minerals present. The balance that is desired is that the mean computed M_NPHI for a given mode is equal to the mean wireline log NPHI (G_NPHI) value for that mode. Here, the G in the mnemonic is a proxy for log.

For example, if (M_NPHI – G_NPHI) > 0 for a given mode, then either the modeled porosity is too high or the modeled clay content is too high. Balance might be approached by either substituting some weight percentage of low-grain-density mineral for some high-grain-density mineral (which would decrease the modeled porosity and therefore the M_NPHI) or by subtracting some weight percentage of a clay mineral and adding the same weight percentage of a nonclay mineral (which would also decrease M_NPHI). These changes must be done while preserving close agreement for that mode between the modeled mode GD and the core GD and the agreement between the modeled clay mineralogy and the core XRD mineralogy.

Once balance is approximated for all modes, particularly the modes believed to contain HCs, then confidence exists that resulting porosity calculations are reliable. Of course, the computed porosities should also match any core-derived porosities, and this is part of the porosity balance requirement discussed above.

The PEF balance, although not essential to the computation of porosity and Sw, is useful for adding credibility to the mineralogic modeling. This is particularly true in gas shales that contain the iron-bearing minerals ankerite, pyrite, and siderite. Although most silicate minerals (quartz, feldspars, most clay minerals) and dolomite have PE values that range from about 1.9 to 3.5 b/e, many gas shales also contain calcite (5.2 b/e) plus the iron-bearing minerals ankerite (~9.2 b/e), pyrite (17 b/e), and siderite (~18 b/e). Because calcite and these iron-bearing minerals can cause significant excursions in the PEF curves, the PEF log is a powerful tool for helping to decipher mineralogic heterogeneity. Modeling is done in a similar manner as that for M_RHOB and M_NPHI, with PEF response for all solid components and all fluid components considered (Appendix H).

Provision is made within forward modeling to model GR and DT, but we have not yet used these in gas shale analyses. The GR is extremely difficult to model, even in conventional reservoirs, because the mineralogic sources and amounts of K, U, and Th are generally poorly known.

Elemental Capture Spectroscopy Versus Forward Modeling Balance: Grain Density and Total Clay Minerals

Although not used quantitatively in the analysis example given below, it is possible (when an Elemental Capture Spectroscopy [ECS\textsuperscript{TM}, manufactured by Schlumberger] or equivalent nuclear spectroscopy is available) to strive for balance, for each clustering mode, between (1) GD from ECS analysis and GD from
forward modeling and (2) weight percent total clay minerals from ECS analysis and weight percent total clay minerals from forward modeling. The inclusion of these balances adds significant rigor and credibility to the forward modeling.

**Kerogen Balance**

The ECS analysis does not permit an estimation of kerogen. However, it is possible to strive for balance, for each clustering mode, between kerogen from profiles derived from core analyses and kerogen used in forward modeling. This is particularly useful because of the significant impact of the low-density kerogen on the modeled bulk density of the samples.

**Water Saturation Balance**

Two basic controls are placed on Sw. One is that Sw must be between 0.0 and 1.0, and the other is that in wet rocks (no HCs present), the resistivity of water-saturated rock (Ro) is similar to true resistivity (Rt) (Ro ~ Rt). The latter constraint is the more difficult to evaluate in conventional reservoirs, and in gas shales, it can be even more difficult to evaluate because of the difficulty of recognizing intervals that contain no gas. Evaluation requires a computation of true conductivity (Co) and its inverse: the resistivity of water-saturated rock (Ro). The method we use is described in Appendix B.

**Estimating Free Gas Gross Pay**

In conventional reservoirs, gross pay original gas in place (OGIP) is commonly computed using Sw and TPOR.

\[
OGIP = k(Shc)(TPOR) = k(1 - Swt)(TPOR) \quad (15)
\]

(from Sustakoski and Morton-Thompson, 1992)

where

- \( Shc \) = hydrocarbon saturation (fractional)
- \( Swt \) = total water saturation (fractional)
- \( TPOR \) = total porosity
- \( k \) is a constant that incorporates reservoir area and thickness, a reservoir HC (compression) factor, and a conversion factor (to generate results in acre-feet)

Although this method can be used in gas shales, the use of TPOR could be misleading because it incorporates a large component of BPOR. Although it might be tempting to use EPOR in conjunction with Swt, the computation of OGIP using EPOR can result in underestimation of OGIP by amounts approaching 50%. This is explained in the following discussion.

The EPOR should be used in conjunction with Swe. Assuming that IPOR cannot contain HCs, Swe is defined as

\[
Swe = (IPOR + FPORW)/EPOR \quad (16)
\]

To obtain Swe, begin with the Swt

\[
Swt = (BPOR + IPOR + FPORW)/TPOR \quad (17)
\]

Rearrangement and substitution gives

\[
Swe = [(Swt)(TPOR) - BPOR]/(TPOR - BPOR) \quad (18)
\]

And, if bound Sw (Swb) is defined as

\[
Swb = BPOR/TPOR \quad (19)
\]

then

\[
Swe = (Swt - Swb)/(1 - Swb) \quad (20)
\]

and

\[
OGIP = k(Shc)(EPOR) = k(1 - Swe)(EPOR) \quad (21)
\]

If OGIP is computed using EPOR and Swe, the same values are generated as when OGIP is computed using TPOR and Swt, that is,

\[
(TPOR)(1 - Swt) = (EPOR)(1 - Swe) \quad (22)
\]

The right side of the above identity is the left side after normalization to remove BPOR. In other word, EPOR and Swe are recomputations of TPOR and Swt after mathematically removing BPOR from the system. The above identity (equation 22) is equivalent to

\[
(TPOR) - (TBVW) = (EPOR) - (EBVW) \quad (23)
\]

where

- \( TBVW \) = total bulk volume water = (TPOR) (Swt)
- \( EBVW \) = effective bulk volume water = (EPOR) (Swe)

In equation 23, both sides of the equation represent the volume of gas present, and the volume is the same on both sides of the equation.

Use of the combination of EPOR and Swt underestimates OGIP. This can be seen in Figure 2. For
example, the black dashed and black solid circles on the green lines for TPOR = 0.10 show that using the combination of EPOR and Swe at BPOR = 0.02 results in about 25% more OGIP than the combination of EPOR and Swt. The percentage difference becomes larger with higher values of BPOR. At BPOR = 0.04, OGIP is about 67% higher using EPOR and Swe than it is when using EPOR and Swt (see brown dashed and brown solid circles at BPOR = 0.04).

So, for reserves estimation, it does not matter which combination of porosity and saturation is used, so long as both terms are consistent (total or effective), but use of TPOR is misleading in terms of the absolute storage capacity of the reservoir.

**Nuclear Spectroscopy Analysis**

Results from a nuclear spectroscopy log, such as Schlumberger’s ECS, in conjunction with standard logs, can be used to generate profiles for TPOR, Swt, and permeability (Herron et al., 2002). The ECS log captures a continuous profile for the elements Si, Ca, Fe, S, Ti, and Gd. Aluminum is estimated using the Si and Fe results. The Si, Ca, Fe, S, and Al are used to estimate mineralogy, and from the mineralogy, the GD is computed (Herron and Herron, 1996).

The advantage of using the ECS log is that a continuous chemical log is generated that directly bears on the mineralogy. Although this is not as good as having a core from which the mineralogy can be determined, it is much better than trying to derive the mineralogy from standard well logs. Modeled mineralogy using an ECS log can be compared with mineralogy modeled using the forward modeling procedure previously described. Spears and Jackson (2009) used this approach in a study of a well in the Barnett Shale where they generated both a volumetric mineral model independent from neutron spectroscopy input and a neutron spectroscopy-based mineral model.

A constraint on using the ECS log (compared with the forward modeling procedure, for instance) is the necessity of making some assumptions during the estimation of mineralogy from chemistry. Specifically, decisions must be made about how to partition the measured elements among the several minerals that can contain those elements.

1) All clay minerals are modeled as a group, as simply clay minerals. This can result in difficulties because all clay minerals do not have the same log response. Similarly, all carbonate minerals (calcite, dolomite, ankerite, siderite, etc.) are modeled as a group. And the silicates quartz and feldspars are modeled as a group.
2) Because the ECS tool does not measure the common elements, Na or Mg, no unambiguous way exists to model minerals in which these elements occur (albite, dolomite, ankerite, etc.).
3) ECS logs do not detect phosphorous, so phosphorous-containing phases cannot be modeled.

The developers of the ECS chemistry-to-mineralogy procedure (Herron and Herron, 1996) acknowledged the problems with attempting to model multimineral rocks without having downhole data from all major elements and expressed the wisdom of calibrating the inputs into their default equations using core mineralogy analyses. To help overcome some of the above difficulties, we commonly use the output of the mineral types from the forward modeling procedure to aid some of the ECS calculations, such as estimating GDs for the clay group, carbonate group, and quartz-feldspar group, and for estimating a likely CEC.

Because both the forward modeling and ECS procedures have advantages and disadvantages relative to one another, we generally use both whenever an ECS log has been run. Because similar results should be reached using both methods, use of both models permits a cross-check between the two methods so that adjustments can be made in inputs as justified. In the example (see below), we show some of the output from the complementary ECS analysis, but do not discuss the workflow in any detail.

**Adsorbed Gas**

In gas shales, a fraction of total gas in the reservoir is adsorbed to the matrix as opposed to being free in the pores. Most of this gas is generally assumed to be adsorbed to kerogen, but this assumption may be because of a paucity of detailed study of adsorption onto other matrix components such as clay minerals. The amount of adsorption onto clays in the Barnett Shale is believed to be limited (Bowker, 2007) and, according to Jarvie (2009), that amount is insignificant because the shales are water wet, thereby preventing direct contact of methane molecules to clay matrix materials. However, at least one study has indicated that illite-rich shales have a significant methane adsorption capacity even after moisture equilibration (Hartman et al., 2008).

The basic questions to be answered in terms of adsorbed gas production are these:

1) How much gas is adsorbed?
2) How much of this gas will be released and at what rate?
3) How is the petrophysics handled?
4) Can wellbore pressures be sufficiently drawn down to cause release of adsorbed gas as would be predicted from measured isotherm data from the shale?

**Amount of Adsorbed Gas**

The amount of adsorbed gas is estimated by conducting laboratory adsorption isotherm studies on core samples of known TOC content (Waechter et al., 2004). A sample is heated to remove adsorbed gas, placed in a vacuum chamber at reservoir temperature, and then permitted to adsorb gas introduced into the chamber as the pressure is increased. A plot of adsorbed gas versus pore pressure shows a linear increase in adsorbed gas at low pressures and a gradual flattening of the adsorption amount at higher pressures until the rock is saturated with adsorbed gas where the amount adsorbed asymptotically reaches a maximum. More comments about adsorption are in Appendix E.

Generally, the adsorption capacity at a given pressure increases with TOC content and with decreasing temperature. The gas content is generally given in units of standard cubic feet of gas per ton of rock (scf/ton), a unit that has been adopted from the coal gas industry.

**Petrophysics**

To estimate adsorbed gas, we approximately follow the method previously described by others (e.g., Lewis et al., 2004; Spears and Jackson, 2009). The procedure is outlined in Appendix E.

The method hinges in part on conducting adsorption isotherms in the laboratory of core samples with known TOC content. The adsorption isotherm provides a measure of maximum gas adsorption possible at a given reservoir temperature and pressure. As reservoir pressure drops because of production of free gas, the adsorbed gas will begin to desorb to maintain equilibrium. Any of this adsorbed gas, now desorbed, would essentially become free gas and join the production stream.

To implement the equations that provide in-situ adsorbed gas (see Appendix G), a TOC profile is needed. Various approaches have been used involving selected well logs calibrated to core data parameters such as porosity and TOC content (Passey et al., 1990; Issler et al., 2002).

Typical practice is to compute the free gas content and the adsorbed gas separately and then sum those to obtain the total gross GIP. Then the ratio of adsorbed to free gas that will be produced at any given time during the history of a well will depend on several
factors, but mostly average TOC plus reservoir temperature and pressure.

Because gas shales are typically very heterogeneous and because the science of understanding the desorption phenomena in a producing field is in its infancy, modeling of the adsorbed gas content and the contribution of that gas to production is not straightforward.

EXAMPLE CALCULATION

Data

A vertical well through the Haynesville Formation, northern Louisiana, is used as an example. The Haynesville Formation was interpreted to be at 3337 to 3422 m (10,950–11,227 ft). Two whole cores were taken from the lower parts of the formation.

Standard well logs plus an ECS log were acquired. No image or nuclear magnetic resonance logs were acquired. Routine core analysis (porosity and GD only), pulse-decay permeability, XRD, TOC (wt. %), Rock-Eval, and Dean-Stark pore fluids analysis were available on 18 whole core samples. Mercury injection capillary pressure (Pc) measurements were made on four samples. No adsorption isotherm measurements were available, and no kerogen isolate chemical analyses were made.

Methods

Data and Logistics for Probabilistic Clustering Procedure and Forward Modeling

A variable core-to-log depth correction of +7.0 to +8.5 ft (+2.1 to +2.6 m) was interpreted. Weight percent TOC was converted to weight percent kerogen using a multiplier of 1.20. This multiplier gave the same volume percent kerogen values as those reported in core analyses when a kerogen density of 1.35 g/cc was used and happened to be the same multiplier used by Spears and Jackson (2009) in an analysis of shale-gas wells in the Barnett Shale. Any dolomite, ankerite, and siderite present in the bulk rock were assumed to have been removed before TOC analysis, so TOC corrections were not made for those minerals. Kerogen properties used were density = 1.35 g/cc, CEC = 1 meq/100 g, SA = 100 m²/g, HIn = 0.85 (fractional porosity units), and Pe = 0.17 b/e.

Fluid properties for forward modeling were formation water density and HIn = 1.05 and 0.9, respectively; gas density and HIn = 0.24 and 0.53, respectively; invasion fluids fraction, density, and U = 1.0, 0.9, and 0.5, respectively. Water resistivity was assumed to be 0.030 ohm m at 300°F (149°C). Matrix components used for modeling were quartz, plagioclase feldspar, K-feldspar, calcite, dolomite, ankerite, illite, chlorite, pyrite, and kerogen.

Classification Via Probabilistic Clustering Procedure

A clustering run (10,950–11,227 ft [3338–3422 m]) was made using RHOB, NPHI, GR, DT, and PEF log data, plus weight percent kerogen as clustering variables. This depth range is from the interpreted Bossier-Haynesville contact to the Haynesville-Smackover contact. Twelve modes were used in an attempt to adequately represent the heterogeneity. Inclusion of kerogen as a clustering variable resulted in the generation of a continuous kerogen profile. Modes were interpreted, using GR cutoffs and apparent GD, to be two siltstones (GR < 180), nine shales (GR > 180), and one dolostone (GD ~3.2 g/cc).

Examination of the results indicated PEF response to be better for relating modes to reservoir quality than the other clustering variables, so most modes were color coded into two general groups: green = PEF < 5, and blue = PEF > 5. Most modes with high-PEF samples were interpreted to be rich in calcite. The mode with both high PEF and high GD was interpreted to contain significant iron-rich dolomite (ankerite) and was assigned an orchid color. Examination of whole core strongly suggested that the high-PEF zones were caused by the presence of carbonate beds and not because of barite invasion.

Results

Free Gas

Table 1 shows the generic lithologies assigned to each mode, the percentage of samples assigned to each mode, the apparent GD (from extrapolation of RHOB versus NPHI plots to zero NPHI), and the mean values of wireline clustering variables for each mode. Panels A and B of Figure 3 are plots of RHOB versus NPHI and DT versus PEF. The samples are color coded to the mode with the highest probability assignment. The ellipses are six-dimensional ellipsoids projected onto the xy planes drawn at approximately two standard deviations from the mean of each mode.

Figure 4A shows the kerogen weight percent versus GR for the 18 core samples, and Figure 4B shows the
same plot but includes kerogen values predicted during clustering for all of the other samples. Figure 4C shows RHOB versus kerogen weight percent for the 18 core samples, and Figure 4D shows the same plot but includes kerogen values predicted during clustering for all of the other samples. The modeling results in excellent correlations between kerogen weight percent and RHOB for some of the modes. The modes with the best correlations are M13, the most abundant mode and interpreted to be siltstone, with $r^2 = 0.88$, and M14, the mode interpreted to be a dolostone, with $r^2 = 0.95$.

Panels A and B of Figure 5 are depth plots. The first track in Figure 5A contains GR and caliper logs plus the kerogen content of the 18 core plug samples. Track 2 shows the probabilistic (fuzzy) assignments. Track 3 shows curves for TPOR, EPOR, Swt, and Swe. Data points are also shown for core plug porosity.

**Table 1.** Modes defined by the probabilistic clustering procedure. Information includes general lithologies (Lith) assigned to each mode, the percentage of samples assigned to each mode, the apparent grain density ([GD] from extrapolation of well-log bulk density [RHOB] versus neutron [NPHI] plots to zero NPHI), and the arithmetic means for RHOB, NPHI, gamma ray (GR), interval transit time (DT), and photoelectric factor (PEF). Slt = siltstone; Sh = shale; Ds = dolostone.

<table>
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<th>Mode</th>
<th>Name</th>
<th>Lith</th>
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<th>Color</th>
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<th>NPHI</th>
<th>GR</th>
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<td>11</td>
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<td>sky blue</td>
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<td>4</td>
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<td>Sh</td>
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<td>4.06</td>
<td>14</td>
<td>3.188</td>
<td>2.502</td>
<td>0.200</td>
<td>211.0</td>
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**Figure 3.** (A) Bulk density (RHOB) versus neutron (NPHI). (B) Interval transit time (DT) versus photoelectric factor (PEF). Samples are color coded to the mode name displayed in the legend at top right.
(18 points) and core fluid saturation (8 points). To illustrate results for ECS analysis, EPOR (EPOR_ECS) and Swe (Swe_ECS) are also shown.

The core porosity points generally fall between computed TPOR and EPOR. This is reasonable in light of the tendency for laboratory sample preparation to sometimes lower the intrinsic porosity (but also some questions exist as to how much of the BPOR is detected in the laboratory procedure for measuring TPOR). Core Sw points generally fall between the modeled Swe profile and the modeled Swt profile. This suggests that all of the BPOR was not detected in the laboratory procedures for measuring fluid saturations. Modeling of Swe is very sensitive to inputs, and incorrect modeling in low TPOR ranges can cause Swe to become negative. In such cases, Swe can be increased, for instance, by decreasing the amount of illite, decreasing the CEC of illite, or increasing Rw. This subtle interplay among inputs helps to put constraints on water resistivity (Rw).

Track 3 in Figure 5A shows three estimates of gross pay using arbitrary EPOR and PERM values as cutoffs: red = pay 1 (conservative): EPOR > 0.10, PERM > 0.01 md; blue = pay 2 (nominal): EPOR > 0.08, PERM > 0.001 md; and green = pay 3 (liberal): EPOR > 0.06, PERM > 0.0001 md. The Swe could also have been included as a cutoff.

Track 4 in Figure 5A compares modeled NPHI (M_NPHI) with well-log NPHI (G_NPHI). The M_NPHI is about 4 to 6 porosity unit (PU) too high because of an imposed invasion factor of 100%. Removal of the invasion factor results in a much better match of M_NPHI with G_NPHI (Figure 6). Note that a trend of relatively constant M_NPHI values exists for a given mode. This is the result of the modeling process wherein each mode has been assigned a specific M_NPHI value. The fact that variations of M_NPHI values exist within a given mode is likely caused by the fact that many samples have been probabilistically assigned to more than one mode.

Track 5 in Figure 5A shows the estimated permeability from forward modeling and from ECS along with core pulse decay permeability. Calibration of forward modeling permeability with core permeability was made by setting \( v_i \) (clay permeability factor; cf. Appendix C) to 0.7 for mode 8 and to 0.2 for all other modes. Most forward modeling permeability values are between \( 10^{-4} \) and \( 10^{-3} \) md below 11,300 ft.

**FIGURE 4.** Weight percent kerogen versus gamma ray (GR): (A) Core samples only, and (B) core samples plus values predicted during clustering; and, weight percent kerogen versus bulk density (RHOB): (C) core samples only, and (D) core samples plus values predicted during clustering.
FIGURE 5. (A) Depth (ft) plot showing well logs, clustering results, core data, and modeled data. Track 1: Gamma-ray (GR) and caliper (HCAL) logs plus weight percent core kerogen (KER_WT). Track 2: Clustering results. The horizontal axis is cumulative probability mode assignment. Track 3: Forward modeled total porosity (TPOR); forward modeled effective porosity (EPOR), effective porosity derived from Elemental Capture Spectroscopy (trademark of Schlumberger) analysis (EPOR_ECS); forward modeled effective water saturation (Swe); forward modeled total water saturation (Swt); effective porosity derived from ECS analysis (Swe_ECS); core porosity (CORE_POR) (red dots); core water saturation (CORE_Sw) (green dots); pay flags (red, blue, and green bars); representative adsorbed gas (dashed black line). Track 4: Well-log neutron (NPHI) and forward modeled neutron (M_NPHI). Track 5: Forward modeled permeability (PERM), permeability derived from ECS analysis (PERM_ECS), and core permeability (Core_PERM). Note that Track 5 is a logarithmic plot, but the minor vertical grid lines between decades are not displayed. Track 6: Deep resistivity (AT90) and resistivity of water-saturated rock (Ro). GAPI = gamma-ray API units; C1 = cluster 1.
FIGURE 5. (cont.). (B) This depth (ft) plot shows additional tracks over the same depth range displayed in panel A. This panel shows core and modeled grain density and mineralogy data, crisp clustering results, plus well-log and modeled photoelectric factor (PEF). Track 1: Core grain density (GRNDEN) and forward modeled grain density (RHOG), and pyrite (PYR) from x-ray diffraction (XRD) and forward modeled pyrite (Pyr_w). Track 2: calcite from XRD (CAL) and forward modeled calcite (Cal_w), dolomite + ankerite from XRD (CORE_DOL_ANK) and forward modeled dolomite + ankerite (Ank_w), and ECS total carbonate (CARB_ECS). Track 3: illite + mica from XRD (CORE_ILL_MICA) and forward modeled illite (III_w), chlorite from XRD (CORE_CHL) and forward modeled chlorite (Chl_w), and ECS total clay minerals (CLAY_ECS). Track 4: quartz from XRD (QTZ) and forward modeled quartz (Qtz_w), plagioclase feldspar from XRD (CORE_PLAG) and forward modeled plagioclase feldspar (Plg_w), and ECS total quartz plus feldspar (WQTFSP_ECS). Track 5: clustering results, most probable (crisp) mode displayed. Track 6: well-log PEF (PEFZ) and forward modeled PEF (M_PEF). C1 = cluster 1.
(3444 m). Above that depth, the rocks are much more
heterogeneous, and the permeability varies over at
least four orders of magnitude (10⁻⁵–10⁻¹ md).

Capillary pressure (Pc) measurements were compat-
ible with the very low permeabilities. The four Pc
measurements indicated a mean pore-throat radius
of 0.003 to 0.004 μm, with 90 to 95% of the pore
throats having radii less than 0.01 μm. Gas-water sys-
tem entry pressures ranged between 410 and 770 psi
(3 and 5 MPa) and are equivalent to a gas column
height of 1240 to 2300 ft (378 to 701 m). At 2000 psi
(14 MPa), the equivalent invaded fluid saturation
ranged from 6 to 9%, whereas the Dean-Stark porosities
ranged from 10 to 15%. Our interpretation is that
the 6 to 9% displacement detected by the mercury
Pc tests represents most of the EPOR, and that the
additional porosity detected by Dean-Stark extrac-
tion procedures is a combination of additional EPOR
(connected by the smaller pore throats) plus BPOR,
which has had some bound water removed during
laboratory treatment.

Forward modeled permeability (log 10) versus
EPOR is shown in Figure 7A with data points color
coded to the highest mode probability assignment.
The relative smooth trend in the relationship between
permeability and EPOR is caused by the prediction
model used wherein permeability is computed from
TPOR, GD, and SA (Herron et al., 1998). The samples
in shades of green are the ones belonging to modes
that generally have mean PEF values less than 5,
whereas the samples in blues and orchid belong to
modes that have PEF values greater than 5. This sug-
gests that iron-rich rocks have a higher permeability
than relatively iron-poor rocks. Permeability (log 10)
versus kerogen (modeled using core analyses plus
PCP), shown in Figure 7B, indicates that high-perm
rocks (~iron rich) generally cannot be differentiated
from low-perm rocks (~iron poor) on the basis of
kerogen content.

The resistivity balance between deep resistivity and
modeled Rₚ is shown in Track 6 of Figure 5A. The fact
that Rt is greater than Ro throughout the section (ex-
cept for some of the thin zones of mode 9) indicates
that little, if any, of the section is completely water
bearing with no HC saturation.

Figure 5B, Tracks 1 to 4, compares core and forward
modeling GD and mineralogy. The paucity of core
sampling in some interpreted modes and the apparent
well-log homogeneity represented by the dominant
mode in the lower half of the section puts limits on
how closely the rocks can be calibrated and modeled.
The sensitivity of analysis of the continuous ECS log-
ging to variations in group mineralogies is shown
by profiles for total carbonates (Track 2), total clay
minerals (Track 3), and the sum quartz plus feldspars
(Track 4).

Track 5 of Figure 5B shows the clustering results
displayed to show only the mode with the highest
probability assignment for each sample. This crisp
mode display defines modeled beds with a mini-
mum thickness equal to the digitizing step. A beds-
 thickness-filter can be used as a simple upsampling rou-
tine to eliminate thin beds to aid reservoir modeling
(Eslinger, 2007; Slatt et al., 2008).

The crisp plot (Track 5 in Figure 5B) permits visual
emphasis on the last track (Track 6), which compares
modeled PEF (M_PEF) with wireline PEF (G_PEF).
Very good agreement of M_PEF with G_PEF below
11,075 ft (3376 m) exists, except for two thin mode 14
intervals at 11,110 and 11,122 ft (3386 and 3390 m),
where M_PEF is significantly lower than G_PEF. In
addition, in much of the section above 11,122 ft
(3390 m), M_PEF is lower than G_PEF by as much as
5 units. These high PEF excursions occur mostly in
modes 14, 6, 5, and 8.

Forward modeled PEF (M_PEF) can be matched
closely to the wireline PEF (G_PEF) using two alterna-
tive procedures. One is to assume that 1.5 to 2.0 wt. %
barite (from drilling mud) exists in the rocks with the
high PEF values. The other is to include a speculative
Ba-rich apatite as a mineral during forward modeling
and to adjust the amount of apatite and the amount of
Ba in the apatite to force agreement between M_PEF
and G_PEF.

The EPOR versus TPOR is shown in Figure 8. All
samples fall below the (black) concordance line by 2
to 4 porosity units (PUs), indicating that the range of
BPOR is about 2 to 4 PUs. Mode 7 (dark blue) falls clos-
est to 4 porosity units (PUs), indicating that the range of
modeled PEF (M_PEF) with wireline PEF (G_PEF).

The Swe versus Swt is shown in Figure 9. Most
samples fall below the (black) concordance line with-
in a locus of points where Swe is about 0.2 fractional
units less than Swt. Samples with Swe less than zero
are incorrectly modeled.

The Swe versus EPOR is shown in Figure 10. As dis-
cussed in a previous section, we recommend that these
parameters be generally used for gas shale work instead
of the combination of Swt and TPOR and certainly
instead of the incorrect combination of Swt and EPOR.

The product (EPOR) (1-Swe) is plotted versus the
product (TPOR) (1-Swt) in Figure 11. The samples fall
along a perfect concordance line, indicating that these
products have the same values.
Adsorbed Gas

No adsorption isotherms were available from core in this well, so credible estimations of adsorbed gas were not possible using data only from this well. However, we constructed a model that permits discussion of the methodology outlined in Appendix E. This model is discussed as if real adsorption analyses had been conducted.

Figure 12 shows four adsorption isotherms. Each represents a different core sample that has a known TOC concentration (3.0, 3.5, 4.0, and 4.5 wt. % TOC, respectively). The adsorption experiments were run at reservoir temperature (~300°F (~149°C)) up to 6000 psi (41 MPa). The curves were loosely extrapolated to 10,000 psi (69 MPa). The volume at this 10,000 psi (69 MPa) maximum pressure is the Langmuir volume ($V_l$) (Langmuir, 1918; see also Appendix E). The relationship between Langmuir volume and TOC was derived by plotting $V_l$ versus sample TOC. This relationship is approximately linear and is shown at the upper right inset in Figure 12.

---

**Figure 6.** Modeled neutron ($M_{\text{NPHI}}$) versus well-log neutron ($G_{\text{NPHI}}$) color coded to mode of highest clustering probability assignment. Concordance line is shown (black). Samples are color coded to the mode name displayed in the legend at top right.

**Figure 7.** (A) Modeled permeability (log 10) versus effective porosity (EPOR). (B) Modeled permeability (log 10) versus modeled weight percent kerogen. Samples are color coded to the mode name displayed in the legend at top right.

**Figure 8.** Effective porosity (EPOR) versus total porosity (TPOR). The black line is a concordance line. Samples are color coded to the mode name displayed in the legend at top right.
The Langmuir pressure ($P_L$), shown as open circles at approximately 1000 to 1500 psi (7–10 MPa), represents the pressure at one half the Langmuir volume ($V_L$). The relationship between $P_L$ and TOC was derived by fitting a second-order polynomial between the four data points. This relationship is shown at the lower right inset in Figure 12.

These two derived relationships ($V_L$ versus TOC and $P_L$ versus TOC) of Figure 12 permit $V_L$ and $P_L$ to be computed with depth in the reservoir because the kerogen profile from the PCP was converted into a TOC profile. The resulting $V_L$ and $P_L$ profiles were then corrected for differences between reservoir temperature and the laboratory isotherm temperature using the equations in Appendix E. A constant reservoir pressure of 9500 psi (66 MPa) and a geothermal gradient of 0.022°F/ft was assumed. A pressure gradient could have been imposed, but in this case, it was not. The final correction to account for the difference between TOC content of the isotherm samples and the TOC content of the well-log profile, described in Appendix E, was not necessary because of the relationships already derived by interpolating the isotherm data. The results, shown in track 3 of Figure 5A (dashed black line), are given in units of standard cubic feet of gas per ton of rock (scf/ton). For comparison, 100 scf/ton is equivalent to about 0.22 bcf/ft per mi$^2$.

Note that the representative analysis previously described is ideal in that isotherms were run at the same temperature on four samples of varying TOC content. Had this not been done, the relationship between TOC and $V_L$ and $P_L$ might not have been so nicely developed. In addition, isotherms should be run up to the highest reservoir pressure. In this case, a reservoir pressure of 9500 psi (66 MPa) was used but the isotherms were only run to 6000 psi (41 MPa). The model was constructed deliberately in this manner to illustrate that not only the $P_L$ points had to be extrapolated, but also the position of the isotherm at 9500 psi (66 MPa) had to be extrapolated.

Summarizing, the isotherm method relies on reliable laboratory measurements that span the range
of rock heterogeneity and the pressure-temperature range of the reservoir. Further comments and discussion of this method of estimating adsorbed gas are given in Appendix E.

CONCLUSIONS

A PCP using well logs as variables permits a gas shale reservoir to be classified into multiple electrofacies. If the electrofacies are treated as lithofacies, the probabilistic assignment of each (digitized) sample to each lithofacies permits a model to be generated for a mineralogically complex thinly bedded reservoir. Because the beds are too thin for normal well-log resolution, the model is actually an upscaled realization of the properties of the individual thin beds. This model, if sufficiently calibrated with core data, results in the development of profiles for TPOR and EPOR, Swt and Swe, permeability, plus other parameters.

The estimation of gross free gas reserves should not be done using the combined parameters EPOR and Swt. This combination results in an underestimation of reserves. The combination of TPOR and Swt gives the same results as the combination of EPOR and Swe, but the latter pair is more realistic in terms of storage capacity.

Estimation of EPOR and Swe requires a modeling procedure that considers variable GD and variable clay mineralogy with due attention to the CEC of the clay minerals. In addition, kerogen should be included in the bulk rock model. Because of its relatively low density, its exclusion can significantly affect the total matrix GD results. If credible core permeability data are available for calibration, the estimation of permeability can be done with some confidence using a published procedure that uses grain density, porosity, and matrix surface area as input variables.

The estimation of adsorbed gas is a fairly routine procedure given that a credible TOC profile can be established through the reservoir and that representative gas adsorption analyses have been made on core samples. However, computation of the estimates relies on mathematics adopted from the coalbed methane industry that is unproven for gas shales.

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FIGURE 12. A model used to illustrate how gas adsorption isotherms vary with total organic carbon (TOC) content and to aid the discussion of how desorption can occur during pressure drawdown. Adsorbed gas is measured as scf/ton. The intersection of the curves with the vertical axis at infinite pressure (here, ~10,000 psi [~69 MPa]) is the Langmuir volume, and the Langmuir pressure (Langmuir P) is the pressure at which one half of Langmuir volume is adsorbed (see text).
APPENDIX B: WATER SATURATION

The following describes some key workflow procedures in the implementation of the dual-water equation (Clavier et al., 1977) within the forward-modeling procedure.

The conductivity of bound water \( C_B \) is equal to

\[
BQ_v / S_{\text{wb},\text{ltd}} = B / W
\]

where

\( B \) = the specific counterion conductivity in mho/m per meq/cc, corrected for temperature (\( ^\circ \)C) = (0.03772 \times T) – 0.6516. (Waxman and Thomas, 1974)
\( S_{wb, ltd} \) = bound water saturation limited to less than 1.0; if \( S_{wb, ltd} \) is less than zero, then set \( C_B \) is equal to zero.

The conductivity of the effective water (\( C_W \)) is \( \frac{1}{R_{wc}} \), where \( R_{wc} \) is \( R_w \) corrected for temperature.

The dual water equation contains two terms. The first term is the conductivity of the effective water (\( C_{EPOR} \)), which is equal to \( \frac{1}{R_{wc}} \), where \( R_{wc} \) is \( R_w \) corrected for temperature and any displacement by filtrate fluid. The second term is the conductivity of any clay-bound water that is present. In our forward modeling, this term is denoted as Term C_Dual Water (\( TC_{DW} \)). If no bound water is observed, that is, if \( S_{wb, ltd} \) is equal to (or less than) zero, then \( TC_{DW} \) is set to zero and the equation for \( C_o \) reduces to the first term only.

Using both terms, \( C_o = \left( \frac{C_W}{\text{trial}_F_{\text{Zero}}} \right) + TC_{DW} \),

where
\[
TC_{CW} = [(\text{CB})(S_{wb, ltd})_I((\text{CW})(S_{wb, ltd}))_{\text{trial}_F_{\text{Zero}}}];
\]
\( \text{trial}_F_{\text{Zero}} = \text{the formation factor using M}_{Zero}_{\text{Use}} = \text{Init}_a/TPOR^M_{Zero}_{Use} \) (from the definition of the formation factor);
\( \text{and } M_{Zero}_{Use} = M_{Zero} \) (see section on permeability estimation) multiplied by an \( m \) factor; the \( m \) factor is used for calibration and its default value is 1.0.

Once \( C_o \) is computed, then the resistivity of water-saturated rock (\( R_o \)) is \( \frac{1}{C_o} \). To prevent excessively large values of \( R_o \), a maximum \( R_o \) of 50,000 is used when \( C_o \) is less than 0.0001.

Next, a limited \( R_o \) (\( R_{o, ltd} \)) is computed as follows:

First, a check is made comparing \( \text{trial}_F_{\text{Zero}} \) with \( R_t / R_{wc} \):

- If \( \text{trial}_F_{\text{Zero}} \) is less than \( R_t / R_{wc} \), then \( \text{trial}_F_{\text{Zero}} \) is used in the \( C_o \) equation. Otherwise, \( R_t / R_{wc} \) is set to \( F_{Zero, ltd} \) and \( F_{Zero, ltd} \) is used in the \( C_o \) equation instead of \( \text{trial}_F_{\text{Zero}} \). The rational for this check and selection of a value for \( F_{Zero} \) comes from the Archie equation.

- From Archie, if \( S_{wt} = 1.0 \), then \( F = R_t / R_{wc} \). If \( F \) is less than \( R_t / R_{wc} \), that means that \( S_{wt} \) is less than 1.0, and that is possible. But, if \( F \) is greater than \( R_t / R_{wc} \), that implies that \( S_{wt} \) is greater than 1.0, which is not possible, so the \( \text{trial}_F_{\text{Zero}} \) is not acceptable, and so \( F_{Zero, ltd} \) is used.

Next, a resistivity balance (\( R_{stBal} = R_t - R_o \)) is computed. For water-saturated (tight or nonproductive) rocks (\( S_{wt} \sim 1.0 \)), \( R_{stBal} \) should be close to zero because \( R_o \) should approximate \( R_t \). If \( R_{stBal} \) is positive, hydrocarbons are present. If \( R_{stBal} \) is negative, something is wrong because this is not possible, and so adjustments are required in the modeling inputs.

APPENDIX C: CATION EXCHANGE CAPACITY (CEC) AND CEC PER UNIT VOLUME (\( Q_v \))

Clay minerals affect water saturation calculations for two primary reasons: their effect on electrical conductivity and their effect in reducing effective porosity. Clay minerals contain bound water that contributes to electrical conductivity. Also, clay minerals, if located in pores (instead of being part of the detrital matrix), reduce the total porosity (\( TPOR \)) to an effective porosity because of the amount of pore space occupied by the immobile bound water.

Various methods for accounting for the clay and their electrical and volume effects in shaly sandstones have been reviewed, among others, by Asquith (1989). Older methods estimated clay volumes from some combination of gamma-ray (GR), neutron, or spontaneous potential logs. For instance, a standard procedure for estimating the volume of clay (\( V_{clay} \)) has been to relate a GR log to clay content and then to subtract the volume of this clay from the TPOR to obtain effective porosity. Despite that it is well known that the use of the GR curve for estimating \( V_{clay} \) is very crude and commonly misleading, tradition commonly prevails, and this method of estimating \( V_{clay} \) is still commonly used. For shaly sands that contain phosphatic materials, the high associated uranium or thorium can render disastrous the attempt to use GR as an indicator of clay.

More realistic methods attempt to account for clays using a more sophisticated model of how clay minerals interact with water. Two of these are the Waxman-Smits-Thomas (WST) model (Waxman and Smits, 1968; Waxman and Thomas, 1974) and the dual-water (DW) model (Clavier et al., 1977). Although we use the DW model, both the DW and WST models give similar results if the formation water salinity is not at the extremes of either very fresh or very salty. Neither model requires a direct insertion of a \( V_{clay} \) term. Instead, clay content is related to the cation exchange capacity (CEC) of the clay. The requirement is an insertion of a term, \( Q_o \), that is equal to CEC per unit pore volume. Thus, the CEC must be known, or estimated, and the pore volume must be known or determined.
Reported ranges for CEC (milliequivalents per 100 g of sample) are as follows:

Smectite: approximately 80 to approximately 130 (varying mostly with magnitude and distribution of interlayer charge)
Kaolinite: approximately 1.7 to approximately 3.8 (varying mostly with crystallinity [~crystal size])
Illite: approximately 10 to approximately 40 (Grim, 1968, p. 189), but a more realistic range is probably approximately 23 to approximately 27 (van Olphen and Fripiat, 1979).
Chlorite: approximately 10 to approximately 40 (Grim, 1968, p. 189), but these values are probably all too high and are likely resulting from the analysis of contaminated samples; a value of approximately 2 is probably more realistic (D. McCarty, 2004, personal communication).

**APPENDIX D: PERMEABILITY**

The Herron et al. (1998) method relies on a variation of the Kozeny-Carman equation (Carman, 1956), which relates permeability to surface area. A lambda ($\lambda$) parameter (after Johnson et al., 1986) is used as “an electrical estimate of the size of dynamically connected pores” (Herron et al., 1998, p. 1). In a rock saturated with conducting fluids, the lambda was shown (Johnson et al., 1986) to be inversely proportional to the ratio of the integrated square of the electrical field over the surface area to the integrated square of the electrical field through the pore volume. Assuming that this ratio of electrical fields is proportional to the ratio of (empirically measured) surface area to pore volume ($SA/V_p$), and that $SA/V_p$ is inversely proportional to pore-throat radius, and that pore-throat radius mostly controls permeability, then the lambda is inversely related to permeability.

Herron et al. (1998) provide two equations for two permeability values, $k_{L1}$ and $k_{L2}$, the first for samples with permeabilities greater than 100 md and the second for samples with permeabilities less than 100 md:

$$k_{L1} = \frac{Z_1 \varphi^{m^*+2}}{[\rho_m^2 (1-\varphi)^2 (\Sigma M_i v_i SA_i)^2]}$$

where
- $Z_1 = 88$ (a proportionality factor)
- $\varphi$ = fractional porosity
- $m^*$ = cementation factor
- $\rho_m$ = matrix density
- $M_i$ = mass fraction of mineral $i$
- $v_i$ = clay permeability factor = fraction of clay minerals that act to affect (reduce) permeability (Herron et al. [1998] suggest 0.1 for detrital clays and 0.2 for authigenic clays)

$$SA = \text{specific surface area (m}^2/\text{gm})$$

and

$$m^* = 1.653 + 0.0818 (SA \rho_m)^{0.5}$$

This equation for $m^*$ is from Herron et al. (1998), who derived the relationship from the empirical data in Sen et al. (1990).

The low-permeability equation is:

$$k_{L2} = \frac{(0.037 Z_1^{1.7} \varphi^{1.7/m^*+2})/ [\rho_m^{3.4} (1-\varphi)^{3.4}] \times (\Sigma M_i v_i SA)^{3.4}]}{\lambda}$$

Implementation within the forward-modeling procedure is as follows:

First, $SA_{\text{Bulk Rock}}$ is determined for each mode via mass balance from $SA_{\text{Clay}}$ and $SA_{\text{NonClay}}$. The latter two components are determined via mass balance using the mineralogy assigned to each mode.

Second, $SA_{\text{Bulk Rock}}$ is determined for each sample using the probabilistic clustering procedure (PCP) probabilities:

$$\Sigma (SA_i \times M_{\text{dry, i}})$$

where
- $SA_i$ = surface area for $i$th mode, and
- $M_{\text{dry, i}}$ = dry mass fraction (which is equal to the fractional probability assignment from PCP run)

Third, $SA_{\text{Bulk Rock}}$ is converted to $SA_{\text{eff}}$, because $SA_{\text{eff}}$ is used to compute $m^*$ (Herron et al., 1998). $SA_{\text{eff}}$ is the effective surface area of the bulk rock after being reduced by the clay permeability factor ($v_i$).

To make this conversion, $SA_{\text{eff}}$ is determined for each mode:

$$SA_{\text{eff}} = \Sigma [(SA_{\text{Clay}} \times v_i) + (SA_{\text{NonClay}} \times 1.0)]$$

where $v_i$ can vary for each mode.

Then, the $SA_{\text{eff}}$ is determined for each sample using the clustering probabilities.
Then, \( m^* \) is used, along with \( \text{SA}_{\text{eff}} \), in the computation of permeability.

**APPENDIX E: ADSORBED GAS**

In the text above, the term adsorption is used. Gas can be both adsorbed and absorbed. Adsorption refers to gas that is physically attached to the external surface of the adsorbing media, whereas absorption refers to gas that is chemically attached to the internal surfaces of the absorbing media. Together, they are the sorbed gas (Moore, 1972; Jarvie et al., 2007).

Adsorption is typically assumed to occur because of a monolayer of gas being adsorbed to the surface of the adsorbing media. According to the Langmuir isotherm theory (Moore, 1972), the linear part of a sorption isotherm is caused solely by adsorption and a discontinuity in the slope of the isotherm once all available surface sites are occupied should exist. Additional sorption at higher pressures is manifested by a gradual decrease in the isotherm slope and is attributed to a combination of absorption plus additional layers of gas that are stacked onto the adsorbed monolayer.

The model outlined above assumes that no adsorption occurs until the adsorbed monolayer is complete. This model suggests that an isotherm that lacks a linear low-pressure segment might be adduced to be caused by a combined adsorption and absorption in the low-pressure regime before the monolayer being completed. Also, this model predicts that the first desorbed gases in a reservoir undergoing pressure drawdown would be from any absorbed gases and from adsorbed gases that might be above the adsorbed monolayer.

Further discussion regarding the aforementioned data is beyond the scope of this chapter because of complications such as: (1) different kinds of kerogen have different adsorption properties; (2) different gases (methane, propane, butane, etc.) have characteristic kerogen-gas distribution coefficients; and (3) difficulties with characterization and quantification of external surface area versus internal surface area of kerogen macerals.

The workflow used to estimate the amount of adsorbed content is outlined next.

First, a total organic carbon (TOC) profile is needed through the reservoir. If a sufficient number of TOC analyses of core have been made (sufficient meaning a few analyses from all of the rock types present), it might be possible to establish a relationship between standard well logs and TOC such that a continuous TOC profile can be generated (e.g., Issler et al., 2002). This is an option within probabilistic clustering procedure (PCP) if the desired TOC analyses are available. An alternative option is to develop a well kerogen profile and then convert that profile into a TOC profile. This is the method that we used in the example analysis.

One way to create a kerogen profile is to develop a relationship (calibrate) among standard well logs, a nuclear spectroscopy log, and an interpreted Rock-Eval kerogen content from core samples so that a continuous profile can be generated. Schlumberger does this with the aid of their ELANPlus™ program (R. Lewis, 2008, personal communication). The resulting kerogen profile is in units of volume percent of bulk rock, and this is then converted to weight percent TOC (Herron and LeTendre, 1990):

\[
\text{TOC} = \frac{(\phi_k \rho_k)}{(\rho_b \kappa)}
\]

where

- \( \text{TOC} \) = total organic carbon (wt. %)
- \( \phi_k \) = kerogen (vol. %)
- \( \rho_k \) = kerogen density (g/cc)
- \( \rho_b \) = bulk density (from well-log bulk density [RHOB])
- \( \kappa \) = kerogen conversion factor

The need for conversion from volume percent kerogen to weight percent kerogen is obviated if kerogen is quantified as weight percent instead of volume percent, but a conversion factor is still needed to relate weight percent kerogen to weight percent TOC. The kerogen conversion factor \( 1/\kappa \) above is equivalent to the \( 1/\kappa \) conversion factor, discussed in Appendix F below, which varies with kerogen type and maturity. The conversion factor \( 1/\kappa \) can range between 1.18 and 1.48 (R. Lewis, 2008, personal communication), and in the analysis made in Appendix F (for two Barnett shale samples), it ranges between 1.30 (mature shale) and 1.56 (immature shale). The range of 1/1.18 to 1/1.48 (0.85–0.68) implies that kerogen, by weight, is approximately 68 to 85% carbon.

Gas content (gc) is computed as a function of TOC-corrected reservoir-temperature Langmuir volume (\( V_{lt} \)), reservoir Langmuir pressure (\( P_{lt} \)), and reservoir pore-pressure (p). The \( V_{lt} \) is derived from TOC-uncorrected reservoir-temperature Langmuir volume (\( V_{lh} \)) by normalizing the well-profile TOC to the TOC in the sample(s) used in the laboratory isotherm. Prior to the above computation, \( V_{lt} \) and \( P_{lt} \) are corrected for differences between reservoir temperature and isotherm temperature. These corrections, taken from the coal-gas industry, are from Herron and LeTendre (1990).
The workflow above cascades from the basic equation (Langmuir, 1918) and associated assumptions:

\[ \text{gc} = \frac{V_l p}{(p + P_l)} \]

where

\( V_l \) = Langmuir volume of adsorbed gas at infinite pressure
\( P_l \) = Langmuir pressure at which one-half of the gas (stored at infinite pressure) will have become desorbed
\text{gc} and \text{p} are as above.

Details of the above workflow are being prepared for publication by Lewis et al. (R. Lewis, 2009, personal communication).

**APPENDIX F: KEROGEN AND TOTAL ORGANIC CARBON**

*Kerogen Chemistry and Total Organic Carbon-to-kerogen Conversion*

Although no constant conversion factor exists for converting from weight percent TOC to weight percent kerogen, Jarvie (Jarvie, 2009, slides 93, 94) shows that S₂ hydrocarbon (HC) can be converted to approximate equivalent LECO™ TOC by multiplying by 0.083. This is because HC are approximately 83% C (by weight) and TOC units are in weight percent but S₂ units are in parts per thousand (g/1000 g). The 83% C in HC cited above is an average. The range is approximately 75 to 89%, with most HCs in the 82 to 85% C range (J. Jarvie, 2009, personal communication).

A variation of the same formula was used to convert Rock-Eval parameters to weight percent TOC (Jarvie and Lundell, 2001):

\[ \text{TOC (wt. %)} = 0.083 \ (S_1 + S_2) + 0.10 \ (S_4) \]

where

\( S_1 \) is the yield of free hydrocarbons vaporized at 300°C in mg HC/g rock
\( S_2 \) is the yield of cracked HC between 300 and 600°C in mg HC/g rock
\( S_4 \) is carbon dioxide generated from reaction with kerogen-free carbon at temperatures above the pyrolysis range in mg carbon/g rock.

The above procedures do not permit the conversion of weight percent kerogen to weight percent TOC in that kerogen. To obtain an accurate conversion factor for converting bulk-rock weight percent TOC (in the kerogen fraction) to bulk-rock weight percent kerogen, the amount of kerogen in the bulk rock and the amount of organic carbon in the kerogen is required. Although the latter can be obtained from a chemical analysis of the kerogen isolate, this is rarely done. Nevertheless, this is discussed below and in Appendix E.

Generally, kerogen is mostly C, H, O, S, and N. For instance, a chemical analysis of kerogen from an oil shale from the Green River Formation gave 80.5% C and 10.3 % H (Atwood, 2006, table 1). Thus, TOC = 0.805 × weight percent kerogen, or “The weight percent kerogen in Colorado oil shale can be calculated by dividing the organic carbon value by 0.805” (Atwood, 2006, p. 2).

For example, if a TOC analysis of the bulk rock indicated 5.0% TOC, then weight percent kerogen = 5.0% / 0.805 = (5.0%)(1.24) = 6.2. Thus, for this sample, the multiplicative conversion factor (TOC to kerogen) is 1.24. The converse is that, if weight percent kerogen was known to be 6.2, then weight percent TOC would be computed as (6.2 wt. %)(0.805) = 5.0%.

Ideally (but only if all of the kerogen were HC prone), a Rock-Eval analysis of the kerogen isolate would generate an S₂ peak that is (from the sum of 80.5% C and 10.3% H) approximately 90.8 mg HC/gm kerogen. And, a Rock-Eval analysis of the bulk rock would generate an S₂ peak that is approximately (90.8 mg HC/gm kerogen)(6.2 wt. % kerogen) = (90.8)(.062) = 5.63 mg HC/gm rock. This assumes that all of the kerogen is cracked during the S₂ temperature range.

Two analyses of kerogen from the Barnett shale (Hill et al., 2007), one immature and one mature, after normalizing elements to 100% gave a weight percent C of 64.3 (immature) and 77.2 (mature), and a weight percent H of 7.48 (immature) and 6.85 (mature). This gives TOC-to-kerogen conversion factors of 1.56 (1/0.643) for immature shale and 1.30 (1/0.772) for mature shale.

Generalizing, the TOC-to-kerogen conversion factor is given by:

\[ \text{wt. % kerogen in bulk rock} = \left[ \frac{\text{TOC (wt. %)}}{[(1/ \text{ wt. % C in kerogen isolate}) \times (100/[100 – \text{ wt. % soluble organics}])]} \right] \]

The first part of the second term can only be determined from a chemical analysis of the kerogen isolate. The second part of the second term is needed because a TOC analysis is done on the insoluble part of the bulk rock. If little to no soluble organics is
observed, then the second part of the second term last term reduces to 1.

**Correcting TOC Analysis for Insoluble Carbonates**

The above discussions and suggested methods are prone to error if the samples that are analyzed via LECO™ or Rock-Eval contain carbonates that have not been removed before analysis.

If dolomite, ankerite, or siderite exist in the bulk rock and they have not been removed from the sample before the TOC analysis, the resulting TOC value can be corrected if the amount (wt. %) of these minerals in the powdered bulk rock is known and the stoichiometry of the unremoved carbonate is known. Consider dolomite (CaMg\([CO_3]\)2). Because two moles of C per mole of dolomite exist, if \(x\) weight percent of dolomite is present, the actual TOC value, after correcting for the CO2 that came from the dolomite, could be estimated as:

\[
TOC_{cd} = TOC \left( \frac{(100\% - [\text{x}\%]) \left(2(MW_{CO2}/MW_{dolomite})\right)}{100\%} \right)
\]

where

- \(x\) = weight percent of dolomite in the sample (after acidification to remove calcite)
- TOC = laboratory value from TOC analysis
- TOC_{cd} = TOC corrected for dolomite content
- \(MW_{CO2}\) = molecular weight of carbon dioxide
- \(MW_{dolomite}\) = molecular weight of dolomite

**APPENDIX G: GRAIN DENSITY AND POROSITY**

Nine steps are described below.

1) For the forward modeling procedure, a temperature profile is generated using a linear regression of user-inserted depth and temperature data points. A grain density (RHO) profile is generated from the varying sample mineralogy (discussed in the text). An initial total porosity profile (TPOR) profile (DPHI1) is computed using a density porosity equation using a constant fluid density (RHOF) but using a variable RHO. In this first approximation of porosity, all fluid is assumed to be water:

\[
\text{DPHI1} = (\text{RHO} - \text{RHOB})/(\text{RHO} - \text{RHOF})
\]

2) An initial estimate of \(S_{wt}\) (Init_Swt) is made using the Archie equation and initial values for \(R_w\), \(m\), \(n\), and \(a\). Each of these four parameters are mode dependent; that is, they can be different for each clustering mode. Thus, the clustering probabilities can be used to generate a variable initial \(R_w\) profile. Then, \(R_{wc}\) is computed to correct an initial \(R_w\) (Init_Rw) for temperature using:

\[
R_{wc} = R_{tf} = R\text{temp}(\text{Temp} + 6.77)/(T_f + 6.77)
\]

(cf. Asquith and Gibson, 1982, pp.5 - 6)

where

- \(R_f\) = resistivity at formation temperature
- \(R\text{temp}\) = resistivity at a temperature other than formation temperature
- \(\text{Temp} = Rmf\) Temp = temperature at which resistivity \((R_{temp})\) was measured
- \(T_f\) = formation temperature

3) A gas-to-oil fraction (GOF) is assigned to each mode. A variable GOF profile is then computed using the probability assignments. This GOF is the relative amounts of gas and oil, by volume, at reservoir conditions.

4) An initial fluid density profile (RHOF1) is computed using a three-component mixture of formation water, oil, and gas:

\[
\text{RHOF1} = (S_{wt} \times \text{RHOwater})
+ (1 - S_{wt})(1 - \text{GOF})(\text{RHOgas})
+ (1 - S_{wt})(1 - \text{GOF})(\text{RHOoil})
\]

In this equation, \(S_{wt}\) uses Init_Swt and the assigned constant density values for water, oil, and gas densities. The density (specific gravity) of oil is computed as 141.5 / (API + 131.5). The density of gas is taken from a plot of density versus reservoir temperature and pressure (Schlumberger, 1987, figure 5-17).

5) An invasion factor (Inv_Ftr) is fractional invasion by drilling mud filtrate and is assigned by mode: 0.0 = no replacement of native fluids (native fluids = formation water + gas + oil); 1.00 = total replacement of native fluids. The Inv_Ftr is used to compute RHOF2.

6) A second fluid density profile (RHOF2) is computed using a four-component mixture of formation water, oil, gas, and invaded filtrate:

\[
\text{RHOF2} = (\text{RHOF1})(1 - X_{mf})
+ (\text{RHO mud filtrate})(X_{mf})
\]

where

- \(X_{mf}\) = invasion factor = volume fraction of native fluids displaced by mud filtrate.
7) A second TPOR profile (DPHI2) is computed using the density-porosity equation and using RHOF2 as fluid density. A DPHI1 profile assumes that only (formation) water is in the pores, whereas DPHI2 considers other fluids (hydrocarbons) plus invaded fluids.

8) Mass_Dry is an internal check on the computed grain densities discussed in the text. Mass_Dry is rock mass excluding all porosity components.

\[
\text{Mass}_\text{Dry} = \sum m_{\text{dry},i} = P_i \times RHOG_i / RHOG
\]

where

\( m_{\text{dry},i} \) = fractional matrix sample mass assigned to mode i (dry means exclusive of porosity; i.e., matrix only)

\( P_i \) = probability of mode i (here, the \( P_i \) probabilities are considered to be applicable to the dry system because the RHOGi and RHOG values used have been extrapolated to zero porosity)

RHOGi = grain density of mode i
RHOG = grain density of sample (already computed; see text)

Note that \( m_{\text{dry},i} \) values are used in the computation of SA of each sample.

9) A third TPOR profile can be done by computing the fractional pore volume assigned to each mode and then for each sample, summing these pore volumes over all modes to obtain the wet volume matrix sum (WVMS) and then subtracting from 1.0. The difference is equal to the TPOR.

\[
\text{WVMS} = V_{\text{wet},i} = P_i \left[ \frac{\text{RHOB} - \text{RHOF}_2}{\text{RHOG} - \text{RHOF}_2} \right]
\]

Then, \( \text{TPOR} = 1 - \sum (V_{\text{wet},i}) \)

where

\( V_{\text{wet},i} \) = fractional pore volume of bulk sample assigned to mode i (wet means that porosity is included in the system)

\( P_i \) = probability of mode i \( \sim \) fractional dry volume (dry means that porosity is not included in the system)

RHOB = well-log bulk density
RHOF2 = fluid density for the ith cluster
RHOG = grain density of sample (computed previously using Geologic Analysis via Maximum Likelihood System [GAMLS] mass balance)

The above equation for \( V_{\text{wet},i} \) is derived from:

\[
\text{RHOB} = (\text{RHOF}_2)(\text{TPOR}) + (1 - \text{TPOR})(\text{RHOG})
\]

or

\[
1 - \text{TPOR} = 1 - \left[ \frac{\text{RHOG} - \text{RHOB}}{\text{RHOG} - \text{RHOF2}} \right].
\]

The fractional probabilities (\( P_i \)) are considered to be equivalent to fractional weights. The TPOR is the actual TPOR value used in the forward modeling procedure. \( \text{TPOR} = 1.00 - \text{WVMS} \).

The DPHI2 porosity (simple DPHI equation) and the TPOR porosity (fractional porosity method) should agree closely if the fluid density of each mode is the same. They serve as cross-checks on each other and show the range of porosity change resulting from the range of fluid density supplied to the equations. For example, if one method says that the porosity is 0.25 and the other method says that the porosity is 0.03, a data input problem exists. If one method says 0.05 and the other 0.06, then the data input is okay and the fluid density difference may account for the 1% difference.

APPENDIX H: NEUTRON AND PHOTOELECTRIC FACTOR MODELING

Bulk-rock neutron response (M_NPHI) is computed stepwise (note that we use NPHI interchangeably with TNPH):

A) First, compute the fluid TNPH (TNPHf):

\[
\text{TNPH}_f = \sum \left[ \frac{(\text{vol. frtn of } i\text{th fluid component})}{\text{TNPH} \text{ of } i\text{th fluid component}} \right] \\
\times \left( \frac{1}{C_0} \right) Xmf \\
+ \left( \frac{1}{C_0} \right) \left( 1 - S_{\text{wt}} \right) \left( 1 - \text{GOF} \right) \left( \text{TNPH}_{\text{gas}} \right) \left( \frac{1}{C_0} \right) Xmf \\
+ \left( \frac{1}{C_0} \right) \left( 1 - \text{GOF} \right) \left( \text{TNPH}_{\text{oil}} \right) \left( \frac{1}{C_0} \right) Xmf \\
\times \left( \text{TNPH}_{\text{filtrate}} \right)
\]

where

\( X_{\text{mf}} \) = fractional invasion
\( S_{\text{wt}} \) = total water saturation
\( \text{TNPH}_{\text{water}}, \text{TNPH}_{\text{oil}}, \text{and TNPH}_{\text{gas}} \) are the constant values inserted as inputs to the forward modeling.

Fractional TNPH (HIn) of pure water = 1.00 at all T and P. However, it decreases with increasing salinity
and temperature; for instance, at 200,000 ppm NaCl, 200°F, and 7000 psi (48 MPa), it is 0.90 (Serra, 1984)

The TNPH for gas varies with gas density, temperature, and pressure; it can be estimated using a chart (Schlumberger, 1987, figure 5-17).

The TNPH value for oil is computed as 1.28 × oil density (Schlumberger, 1987, p. 52, equation 5-13).

The TNPH for mud filtrate depends on the composition of the mud filtrate. Unless data exist to indicate otherwise, we use the same value as that used for water TNPH.

GOF = gas-to-oil volumetric fraction. As described in Appendix G above, GOF is the relative amounts of gas and oil, by volume, at reservoir conditions.

B) Second, compute the matrix TNPH:

\[
\text{TNPH}_m \quad (\text{for mode}_i) = \sum (\text{TNPH of min}_i) 
\times (\text{weight fraction min}_i \text{ in mode}_i)
\]

Then, TNPH_m is computed for each sample:

\[
\text{TNPH}_m \quad (\text{of sample } i) = \sum [(\text{prob}_i)(\text{TNPH}_m, \text{mode}_i)]
\]

C) Finally, compute the modeled bulk-rock neutron response (M_NPHI):

\[
\text{M}_\text{NPHI} = (\text{TPOR}) (\text{TNPH}_i) + (1 - \text{TPOR})(\text{TNPH}_m)
\]

The photoelectric response (Pe or PEF) is controlled by the photoelectric absorption index (U) of the rock components. The data used are tabulated mostly from Schlumberger (1985, p.104–105; 1987, p. 47).

For modeling bulk-rock PEF (M_PEF), we use the expression for Pe given in Dewan (1983, p. 110)

\[
\text{Pe} = [(1.0704) \times (\text{U of bulk rock})]/(\text{RHOB} + 0.1883)
\]

The photoelectric absorption index of bulk rock (U_br) is computed first for each mode and then for each sample. The bulk-rock response is a sum of the matrix response and four fluid response terms. These are computed as follows for each mode:

1) \( U_{\text{br}} \) (U for matrix) = (1 − TPOR) (Σ [mineral_i × matrix vol. % dry])

2) \( U_{\text{for water}} \) (U for formation water) = (0.0048) × (salinity) + (0.3889). This equation is from a regression of \( U \) versus salinity \( (r^2 = 0.9987) \) through four data points ranging from a salinity of 0.01 to 200 ppt (Helander, 1971).

3) \( U_g \) (U for gas) = (0.119) (gas den) (Dewan, 1983, p. 112)

4) Assign \( U_o \) (U for oil). Forward modeling uses 0.115 as default. Schlumberger (1987, p. 47) gives 0.11 to 0.12; Dewan (1983, p. 112) gives (0.136) (oil density).

5) Assign \( U_f \) (U for filtrate). Forward modeling uses 0.50 as default. The photoelectric absorption index for fresh water is 0.4 (Helander, 1971).

Combining these with their relative volumetric fractions gives the following for \( U_{\text{br}} \):

\[
U_{\text{br}} = (1 - \text{TPOR}) \times [\sum (\text{mineral}_i \times \text{matrix vol. } \% \text{ dry})] 
+ (U_{\text{for water}}) (S_{\text{wt}}) + (U_o)(S_o) + (U_g)(S_g)(1 - X_{\text{mf}}) 
+ (U_{\text{mf}})(X_{\text{mf}})(\text{TPOR}) (1.0704)
\]

where

\( S_{\text{wt}}, S_o, \text{and } S_g \) are total water saturation, oil saturation, and gas saturation, respectively; and

\( X_{\text{mf}} = \text{an invasion factor (cf. Appendix G).} \)

Then, the PEF for each sample is:

\[
\text{M}_\text{PEF} \quad (\text{of sample } i) = \sum [(\text{prob}_i)(\text{PEF}_\text{mode}_i)]
\]

REFERENCES CITED


Bustin, R. M., A. Bustin, D. Ross, G. Chalmers, V. Murthy, C. Laxmi, and X. Cui, 2009, Shale gas opportunities and challenges, Search and Discovery article 40382,


