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Bulk Volume Reduction of the Kimmeridge Clay Formation, North Sea (UK) Due to Compaction, Petroleum Generation and Expulsion

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Abstract: In this study, the effects of petroleum generation and expulsion on shale porosity is explored by evaluating the compaction of the Kimmeridge Clay Formation (KCF) within the oil window using log data and shale samples from the KCF within the depth and temperature range of ~1.5-5.0 km and 90-157ºC, respectively. Petrophysical properties e.g porosity and pore-size distribution were measured, and permeability was calculated using empirical models based on the measured porosities. Transit-time values from the sonic logs recorded at depths in the wells were the cores were recovered were calibrated against the porosities determined from the core samples. Bulk geochemical parameters e.g., Total Organic Carbon (TOC), Hydrogen Index (HI) were determined. The volume reduction in the KCF within the oil window due to petroleum generation and expulsion, and compaction due to loss of pore space was determined using the geochemical and log derived porosity data emplaced into empirical relations. Porosities above the oil window range from ~15-20%, but decreased to <5% at the end of the oil window. Pore-sizes decrease from ~11 nm to between 6-8 nm at the depth range of 1.5-5.0 km. Permeability decreased from 4.8 nD to ~0.095 nD. The quantitative estimations of volume reduction within the oil window indicate that for ~8.0wt% initial TOC sediment, a bulk volume reduction of 13% of the initial volume is due to oil expulsion, and ~12% is due to loss of pore space.

Key words: Compaction, hydrogen index, mudstone, permeability, pore size distribution, porosity

INTRODUCTION

Decrease in matrix porosity or compaction occurs due to the inelastic grain deformation in response to the continually increasing effective stress with depth. However, at depths >2-3 km and temperatures ~70-100ºC, Skempton (1970), Bjorlykke (1999), Bjorlykke and Hoeg (1997) and Broichhausen *et al*. (2005) reported that compaction also involves dissolution and precipitation of minerals, and that these processes are strongly controlled by temperature and to a lesser extent by variation in effective stress. Dissolution of mineral phases causes porosity reduction and a closer packing of the grain structure (Nygard *et al.* 2004). This implies therefore that non- mechanical processes may also be important during compaction of sediments in sedimentary basins.

But the conventional approaches to shale compaction have generally neglected to take into account volume reduction of organic matter due to petroleum generation and expulsion, which may, in organic rich shales, account for much of the total volume reduction occurring during burial (Larter, 1988). In organic rich source rocks with TOC > 2.5%, organic matter constitutes a significant fraction of the source rock (Goff, 1983); as a result, the organic matter may partially support the overburden stress (Gutjahr, 1983; Palciaukas, 1991). During petroleum generation, the solid phase kerogen is slowly converted to oil and gas and subsequently expelled. Compared with typical mudstones, the compaction of organic rich rocks may therefore be different due to (a) different compressibility and (b) generation and expulsion of petroleum. The net decrease in source rock volume observed during burial may be due to a composite of porosity reduction driven by mechanical and non-mechanical compaction *and* petroleum expulsion. Therefore, if the mechanics of compaction are understood or, by quantitatively analysing the effects of compaction (e.g., porosity), the irreversible nature of shale compaction (Hedberg, 1936; Magara, 1980) can be exploited to assess the extent to which geochemical processes (e.g., hydrocarbon generation and expulsion) have altered the porosity of the sediments and thus estimate the original volume of sediments required to have been compressed to present thickness within the oil window.

In this study, we have used a geochemical mass balance approach based on empirical relations to determine the volume reduction in a unit volume of the KCF using petrophysical and bulk geochemical parameters due to (a) compaction and (b) petroleum generation and expulsion.

Conceptual model of source rock compaction: The quantification of the bulk volume reduction in an organic rich source rock due to conventional porosity reduction and petroleum generation and expulsion is based on a

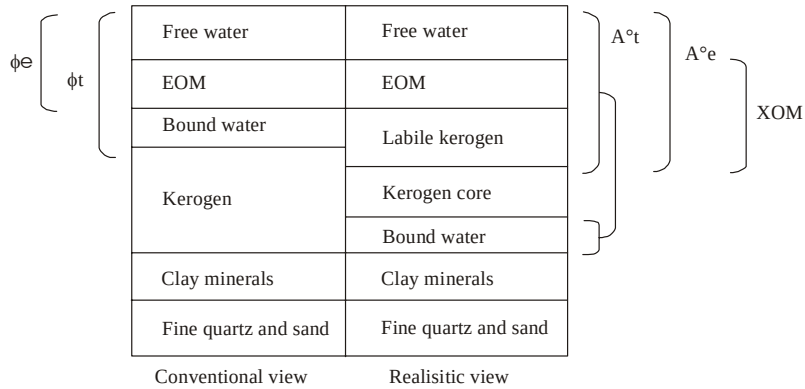

Fig. 1: Source rock versus conventional shales. Volume reduction in organic rich shales during burial may be a composite of conventional porosity reduction and petroleum expulsion (XOM), (after Larter, 1988). Φ_t = is total porosity; Φ_e = effective porosity; A°t =total reducible volume; A°e = effective reducible volume

conceptual model, shown schematically in Fig. 1. The conceptual model is a highly simplified description of the real system that lends itself to a mathematical treatment. A source rock is an organic rich layer of prescribed boundaries of given volume (Vsource), where the organic matter occurs as a network, and has a volume (Vom). The remaining volume ($V_{inorganic}$), is occupied by inorganic solids such as sands, carbonates and clays, and V_Φ, the associated porosity (Fig. 1). In this case, the stress bearing organic matter is not part of the intergranular pore space (Φ) and thus not part of the $V_{inorganic}$, and

$$V_{source} = V_{inorganic} + V_{om} + V_\Phi \quad (1)$$

A realistic compaction model for an organic rich shale is that a significant fraction of the total volume reduction and density increase in sediments resulting from burial, results from major catagenetic conversion of solid phase kerogen to fluid oil and gas, which is partly expelled (Fig. 1). Therefore, by quantitatively evaluating the volume of organic matter in a unit volume of source rock and the associated porosity change before and after petroleum generation and expulsion, the net volume reduction in the source rock can be determined.

MATERIALS AND METHODS

Twenty-two shale core samples from 15 wells taken from the central and northern parts of the North Sea and the Norwegian Margin were selected for porosity measurement. The main sampling criterion was sample quality, since high-quality core material is a prerequisite for the accurate determination of very low porosities. The samples were taken from a depth range of ~1.5-5.0 km, and bottomhole temperature data range from 44-157ºC. Aiming to determine the petrophysical properties of the organic rich KCF, we sampled uniquely from zones with a gamma ray signal over 100API units. Only data from intervals with gamma-ray values >100API units, transit-time values >70 µsec/ft and a relative decrease in bulk density values were chosen. Consequently, data from thin sand intervals within the KCF was screened out. Samples were ground, and organic carbon contents (TOC) were determined using a LECO RLS-100 Carbon-Sulphur Analyser. Bulk pyrolysis parameters were obtained by Rock-Eval pyrolysis (Espitalie *et al*., 1977).

Pore-size distribution of the mudstone specimens was determined by mercury intrusion porosimetry, following the procedure described by Issler and Katsube, (1994). Approximately 5-10 g fragments were cut from the 22 mudstone core samples. Samples were dried first at room temperature and then for 24 h at 105ºC. There was no visible alteration of sample integrity resulting from the cutting or drying procedure. In principle, the mercury porosimeter can generate pressures high enough to force mercury into all accessible pores and measure the volume of mercury taken up by them (Rootare, 1970). Assuming cylindrical pore shapes, the Washburn equation (Rootare, 1970) relates the amount of pressure, p, required to force mercury into pores with pore-size diameter, d, greater than or equal to:

$$d = \frac{-4\gamma\cos\theta}{p} \quad (2)$$

where γ is the surface tension of mercury, and θ is the contact angle. Values of $\theta = 141^o$ and $\gamma = 0.48$ N/m were used in this study. The measurements were made using a Micrometrics Autopore II 9220 mercury porosimeter with an available pressure range of 0.021-269 MPa. The mercury injection pressure was incrementally increased from 0.021 to 269 MPa in 56 pressure steps, and the volume of mercury intruded for each step measured.

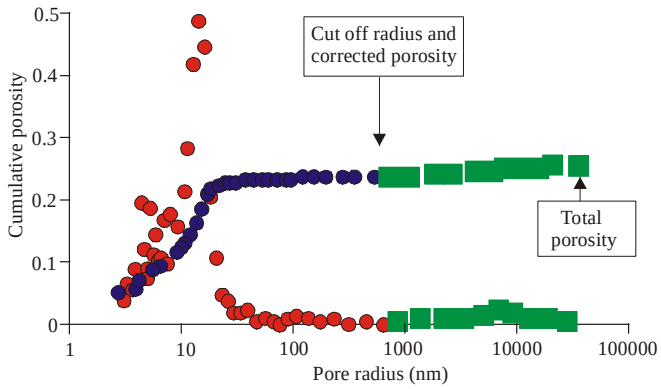

Fig. 2: Example of pore-size distribution. The blue plot marks the cumulative porosity against pore size distribution. The red plot marks the pore density against the pore size distribution

Knowing both the applied pressure and the incremental volume of mercury intruded into the sample allows pore-size distributions throughout the sample to be calculated from Eq. (2). The mercury porosimetry data for this study was taken from Jokanola (2003). The total porosity was calculated from the dry bulk density and the measured grain density. The dry bulk density was calculated from dry weight and bulk volume given by the mercury intrusion. Since sampling and unloading may induce some microfracturing, the total porosity was corrected using pore size distribution data. The approach, illustrated in Fig. 2, is to determine the point at which the pore size frequency curve, when plotted as a function of increasing pore radius becomes a minimum. It is assumed that pores above that "cutoff" radius are sampling artefacts and are removed from the data set.

The mean pore throat radius was calculated for all pores smaller than the cut off radius. It was calculated incrementally from the relative pore size distribution using the equation (Yang and Aplin, 2007):

$$\bar{r} = \sum_i \left(\phi_{\%,j} - \phi_{\%,j-1}\right) \exp\left(\frac{\ln(r_{i-1}) + \ln(r_i)}{2}\right) \quad (3)$$

where, r_i is the pore throat radius at data point *i(nm)*, ϕ% is the fractional relative porosity at pore throat radius and is defined as:

$$\phi_{\%,j} = \frac{\phi_{cum,j}}{\phi_c} \quad (4)$$

where $\phi_{cum,j}$ is the fractional cumulative porosity at data points and is the corrected porosity. In the calculation of mean pore throat radius using above equations, pores smaller than the smallest measured pore (3.0 nm in this work) were neglected since their contribution to the mean pore throat radius is insignificant. The shale porosities were calibrated against transit time values from the sonic log recorded at depths in the wells where the cores were recovered. The porosity-transit time relationship obtained from the calibration is:

$$\Phi = 1 - (66.8/\Delta t)^{1/3.31} \quad (5)$$

where f and Dt are the shale porosity and transit-time respectively. Permeability was modelled from the pore throat size distribution and porosity data using the approach of Yang and Aplin (1998).

As organic matter is slowly converted to oil, the oil is squeezed out of the organic matter and into the pore space (Palciaukas, 1991). During this process, the volume of oil expelled from the source rock is approximately equal to the net decrease in volume of the organic matter, i.e., ΔV_{om}. The volume decrease due to organic matter conversion is temperature induced and occurs only within the oil window. Also, compaction of pore space, ($\Delta\Phi$), due to increasing effective stress or non-mechanical process results in an additional volume decrease. However, the volume of inorganic solids is assumed to be constant. The change in source rock volume in response to passing through the oil window can thus be written as:

$$\Delta V = V_{inorganic} + \Delta V_{om} + \Delta V_{\Phi} \quad (6)$$

where,

V_{matrix} = Volume of inorganic solids (assumed to be constant)

Δ_{vom} = Volume of oil expelled from the source rock and change in kerogen volume

ΔV_{Φ} = Volume change due to compaction of pore space

We have used a geochemical mass balance approach based on empirical relations to determine the volume reduction in the KCF due to petroleum generation and

expulsion. In this approach, we determine the mass of petroleum generated and expelled by determining the decrease in kerogen volume (Cooles *et al*., 1986). The volume percent of kerogen (initial and final) was calculated using the approach of Tyson (1995). The following empirical relations were used:

Initial OM (wt%) =
$(TOC_{initial}$ / wt % carbon of kerogen) * 100 (7)

Present OM (wt%) =
$(TOC_{present}$ / wt % carbon of kerogen) * 100 (8)

Initial kerogen volume (%) =
(Initial OM (wt%) / Kerogen density)
* mineral density (9)

Present kerogen volume (%) =
(Present OM (wt%) / Kerogen density)
* mineral density (10)

Assuming a source rock volume of 1000 m^3

Initial volume of kerogen (m^3) =
(Initial volume of kerogen (%)/100) * 1000 (11)

Present volume of kerogen (m^3) =
(Present volume of kerogen (%)/100) * 1000 (12)

where,
TOC = Total Organic Carbon (wt%)
HI = Hydrogen index (mgHC/gTOC)
Vol. of pet generated (m^3)
= Initial volume of kerogen - Present volume of kerogen
Vol. of petroleum expelled
= Volume generated * expulsion efficiency
Vol. reduction in OM
= Initial volume of kerogen - Volume of petroleum expelled

Expulsion efficiency =

$$[(S_{2(initial)} - S_{2(obs)} + S_{1(initial)}) - (S_{1(obs)}) / (S_{2(initial)} - S_{2(obs)} + S_{1(initial)})] \times 100 \quad (13)$$

where,
Obs = observed
Expulsion efficiencies were determined from pyrolysis data

The volume decrease in the KCF due to compaction of pore space is evaluated using the following relation.

$$V_o = V * (1-\phi/1-\phi_o) \quad (14)$$
$$\Delta V = V_o - V \quad (15)$$

Note that the solid volume is assumed to be constant.

where,

V_o = Original volume of source rock
V = is the assumed present volume of source rock (1000 m^3)
ΔV = amount of compaction
ϕ_o = the initial porosity (%)
ϕ = final porosity (%)

The volume of oil generated from a unit volume of source rock is related to the amount, type and maturity of its kerogen. The subsequent expulsion of the generated oil is related to the expulsion efficiency of oil from the source rock. To quantitatively determine the net volume reduction in the KCF occasioned by petroleum generation and expulsion and compaction (pore space loss), we have assumed a unit volume of the KCF (1000 m^3 source rock volume). We have also carefully chosen two wells (204/27A-1 and 3/29a-4) and reference depths 2800 and 4742 m in these wells corresponding to ~90-151ºC to represent the beginning and end of the oil window. This maturity range was further subdivided into four maturity slices. In each maturity slice, the initial and final volume of kerogen was determined using bulk geochemical parameters (e.g., TOC, HI, kerogen density etc.) and emplacing them in mass balance equations 7-10 so as to determine the volume loss due to petroleum generation and expulsion. The difference between the initial and final volume of kerogen is a measure of the amount of petroleum generated and expelled. Pore space loss and thus volume reduction due to mechanical compaction is determined using the porosities at the respective depths in the wells chosen using Eq. (14) and (15).

Since the KCF does not extend up to a depth of 2800 m in well 204/17A-1, we have used a porosity of 15% at the onset of petroleum generation taken from well 25/2-6 at a depth of about 3100m. Also, the TOC in the immature KCF varies between 6-9 wt%, we thus used an average value of 8.0 wt %. In well 3/29a-4, a TOC value of 4.5 wt % is used, porosity at depth 4742 m varies from ~4-6%. We have decided to use an average value of 5%. Basic petrophysical and geochemical data and results of the volume reduction calculation are shown in Table 1. Below is an illustration of the volume reduction calculation within the maturity range 90-151ºC.

Beginning of the oil window
Maturity 90ºC (Depth: ~2800 m)

Initial TOC	= 8.0 wt %
Initial wt% of kerogen	= 10.7 wt %
Initial volume of kerogen (%)	= 23.5%
Initial volume of kerogen (m^3)	= 235 m^3
Porosity	= 15%
Volume of pore space	= 150 m^3
Volume of minerals	= 615 m^3

Table 1: Petrophysical and geochemical data

Well name	Depth (m)	Temp (ºC)	TOC (%)	HI (mgHC/ gTOC)	Kerogen density (g)	Grain density (g)	Porosity (%)	Mean radius (nm)	Permeability (nm)
31/2 - 2	1515	52	4.16	277	1.23	2.69	24.2	13.5	4.800
35/11 - 4	1979	56	4.03	n.d	1.23	2.69	9.5	14.3	1.400
31/4 - 10	2007	76	5.91	358	1.20	2.67	11.0	7.8	0.870
31/4 - 9	2117	77	9.53	n.d	1.22	2.61	20.5	6.1	1.600
31/4 - 6	2132	79	7.05	357	1.23	2.64	19.2	6.3	1.500
34/10 - 18	2352	60	5.61	406	1.22	2.67	16.4	34.5	7.300
30/9 - 10	2755	75	3.69	n.d	1.23	2.70	16.5	35.6	8.600
30/9 - 14	2978	78	3.06	n.d	1.23	2.86	10.3	6.3	0.640
211/12A - M1	3125	97	8.21	287	1.21	2.64	14.3	13	2.100
211/12A - M1	3282	102	5.81	138	1.24	2.30	15.2	12.7	2.300
211/12A - M16	3376	102	9.77	138	1.24	2.65	24.3	10.9	3.800
211/12A - M16	3401	103	8.18	121	1.22	2.69	23.8	15.7	5.500
34/8 - 6	3578	98	9.43	315	1.21	2.61	12.8	2.3	0.290
16/7b - 20	3932	96	7.53	393	1.22	2.63	9.3	1.2	0.095
16/7b - 20	4030	104	7.42	n.d	1.24	2.65	10.5	2.2	0.081
16/7b - 28	4120	106	8.34	250	1.25	2.64	7.2	2.9	0.180
16/7b - 20	4134	106	11.10	250	1.25	2.62	8.0	3.8	0.270
16/7b - 20	4158	102	5.85	259	1.27	2.62	5.2	2.5	0.100
3/29 --2	4608	130	6.91	38	1.38	2.67	6.4	3.2	0.170
3/29a - 4	4707	141	4.46	48	1.36	2.68	4.3	2	0.067
3/29a - 4	4742	142	6.37	38	1.35	2.67	4.8	2.5	0.095
3/29a - 4	4781	144	6.16	65	1.35	2.66	3.3	4.3	0.100

End of oil window
Maturity 142ºC (Depth: ~ 4742m)

Present TOC (wt %)	= 4.5 wt %
Present wt % kerogen	= 5.0 wt %
Present volume of kerogen	= 10.2%
Present volume of kerogen (m^3)	= 101.9 m^3
Porosity	= 5%
Volume of pore space	= 50 m^3
Volume of solids	= 615 m^3
Calculations	
Volume of oil generated	= 133 m^3
Expulsion efficiency	= 98%
Volume of oil expelled	= 130 m^3
Volume of sorbed oil within the kerogen	= 2.7 m^3
Volume reduction due to petroleum generation and expulsion	=13.04% (of the initial bulk volume)
Volume reduction due to porosity loss	= 11.8% (of the initial bulk volume)
Total volume reduction due to oil expulsion and compaction of pore space	= 23.04% (of the initial volume)

Note: Kerogen densities used in determining the initial and present volume of kerogen in a maturity slice was obtained from Okiongbo *et al*. (2005), while weight percent carbon used for the volume of organic matter estimations in a maturity slice was taken from Rullkotter *et al*. (1988), and a mineral density of 2.75g/cm^3 (Hermanrud *et al*., 1994) was used.

RESULTS AND DISCUSSION

Total organic carbon ranges from 3.4 to 9.8%, mainly between 4 and 9.8% (Table 1). Hydrogen Index (HI) values of the immature samples vary from 260 to 530 mgHC/gTOC, with most samples showing values between 300 and 400 mgHC/gTOC. At temperatures between 100 and 150ºC, petroleum generation and expulsion is reflected in a reduction in HI from 250 to 450 mgHC/gTOC to less than 50 mgHC/gTOC. The reduction in HI occurs mainly over a depth range between 3500 and 4500 m.

The data set is presented in Table 1 and shows that pore throat sizes and porosity range from ~3.0-1000 nm and ~3.0-24%, respectively. The pore size distributions show that the mudstones are characterised by unimodal pore sizes with modes decreasing from ~15 nm at 1515 m to ~6-8 nm as depth increases to 4781 m. Generally, the sample suite is characterised by larger porosities and pore sizes at shallow depth but decreases from ~15 nm at about 24% (1515 m) to ~1.2-5.0 nm at porosities <10% suggesting that with increasing effective stress, porosity is lost by the collapse of relatively larger pores, resulting in a decrease in the mean pore throat size (Yang and Aplin, 1998). Table 1 shows that mean pore radius is almost constant at values <5.0nm suggesting a state of maximum compaction as the porosity approach a critical value of <10%. This reaffirms the fact that most of the porosity loss occurs through the collapse of pores larger than 10 nm (Yang and Aplin, 1998). A lower limit of ~3.0 nm pore radius was determined at a pressure of 269 MPa in all samples. Since mudstones contain pores with radii smaller than 3.0 nm and/or have pores which are not connected to the flow system, the pore size distributions do not start at zero porosity but a porosity which represents difference between the total porosity and that measured by mercury intrusion. Porosity values determined using the correlation function obtained by regressing core porosity values against transit time values

Table 2: Volume reduction through petroleum expulsion and compaction in a unit volume of the Kimmeridge Clay Formation

Well name	Depth (m)	Temp. (ºC)	HI (mgHC /gTOC)	Porosity (%)	Init. TOC (wt %)	Present TOC (wt %)	Vp (%)	Vo (%)	Net vol loss (%)
204/27A-1	2043	90	424	11 - 20	8.0				0.0
25/2-6	3150	100	236	12 - 14	8.0	6.85	5.30	2.4	7.7
3/29a-4	4707	141	36	5.0 - 7.0	8.0	4.80	12.10	10.6	22.7
3/29a-1	4742	142	36	4.7 - 7.0	8.0	4.50	13.04	11.8	24.8

Vp = volume loss due to petroleum generation and expulsion expressed as a percent of the initial volume
V_Φ = volume reduction due to pore space loss as a percent of the initial KCF volume

are consistent with published mudstone/shale porosity versus sonic transit-time data from the North Sea Malm (Kimmeridge) shales thus affirming the validity of the equation.

The equation is able to account for the curvilinear relation between porosity and sonic transit time over a wider porosity range. The equation offers a significant improvement over the widely used time average equation in that porosities derived from sonic transit time values using the transform show a satisfactory fit with those determined experimentally.

Modelled permeabilities range between 9.5×10^{-23} - 8.6×10^{-21} m^2 (8.6-0.095 nD). This range is within that reported by Neuzil (1994) for permeabilities determined both experimentally and inferred for field settings by inverse analysis of pressure or flow data. Table 1 shows an overall decrease in permeability from 8.6×10^{-21} m^2 (8.6 nD) to 9.5×10^{-23} m^2 (0.095 nD) at a depth and porosity range of 1515-4781 m and 3.0-24%, respectively, a decrease of about three orders of magnitude.

We have explored the volume reduction in the KCF through both petroleum generation and expulsion, and loss of pore space due to compaction (assuming only vertical compaction). Petrophysical and geochemical data derived from the KCF only was used (Table 1). The results of the bulk volume reduction estimation are shown in Table 2 and Fig. 3. The results show that for ~8 wt % initial TOC sediment, a bulk volume reduction of ~25% is evident through the oil window of which 13% of the initial volume of the KCF is due to petroleum generation and expulsion. The results also show that a bulk volume reduction of ~12% of the initial volume within the oil window (~2800-4742 m) is through porosity loss. Comparison between percentage pore space loss and volume reduction due to petroleum generation and expulsion indicates that volume reduction occasioned by petroleum generation and expulsion is ~1.2% greater in magnitude than that due to pore space loss.

These results are at odds with theoretical considerations of Palciaukas (1991) who suggested that the bulk volume reduction in oil prone source rocks due to petroleum generation and expulsion is ~4-8 times larger than volume loss due to porosity loss. This discrepancy is from the fact that Palciaukas (1991) has assumed a matrix porosity (Φ) of about 0.05-0.10 around the oil window, and has assumed that the porosity change ($\Delta\Phi$) is not more than 0.02 through the oil window. We have

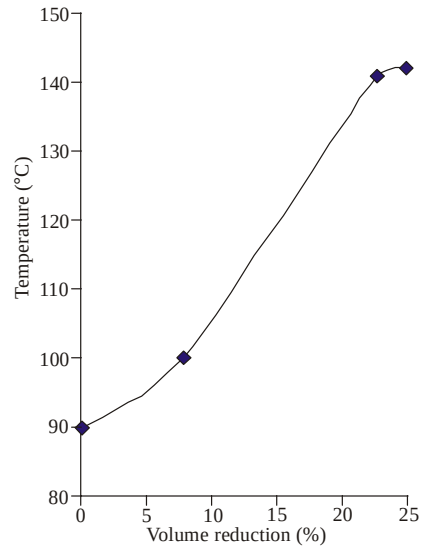

Fig. 3: Net volume reduction in the KCF through petroleum expulsion and loss of pore space

observed in our study that the matrix porosity (Φ) ranges from ~0.03-0.05% to 0.15-0.20% in the oil window in the KCF. We estimated a porosity change ($\Delta\Phi$) of around ~0.75-0.80 in the oil window. Thus the estimated porosity loss in this study is larger than that theoretically considered by Palciaukas (1991). However, the percentage volume reduction (~13%) due to petroleum generation and expulsion is consistent with that (~10%) suggested by Larter (1988) and Palciaukas (1991). The volume reduction estimations in this study are based purely on normal compaction when fluid expulsion is efficient. On the contrary, if expulsion is poor, pore fluids will have considerable difficulty in migrating through the connecting/storage pores. This would result in fluid entrapment, and overpressure within the shale would occur, inhibiting compaction. Also, if the shale grain framework protects the pore spacing from collapsing, porosity will be considerably enhanced and preserved due to transformation of the solid organic matter to fluid, and subsequent expulsion.

CONCLUSION

Mercury porosimetry measurements for 22 mudstone core samples from 15 North Sea wells show a broad range

of pore-size distribution and variation of porosity values. Generally, pore-size distributions of the samples exhibit unimodal distributions with modes decreasing from ~15 nm at 1515 m to ~6-8 nm as depth decreases to 4781 m. The small pore sizes of these mudstones provide a qualitative explanation for the low mudstone permeabilities and why they tend to form reservoir seals. The sonic transit time-to-porosity transform offers an empirical approach to regional porosity determination in the organic rich Kimmeridge Clay Formation in the North Sea basin in that porosity values determined using the correlation function are consistent with published mudstone/shale porosity versus sonic transit-time data from the North Sea Malm (Kimmeridge) shales thus affirming the validity of the equation. Quantitative estimations of volume reduction in the KCF within the oil window indicate that for ~8 wt % initial TOC sediment, a bulk volume reduction of 13% is evident through the oil window simply due to oil expulsion, while a bulk volume reduction of ~12% was estimated as that due to mechanical compaction. In comparison, the bulk volume reduction due to petroleum generation and expulsion in organic rich shales is ~1.2% greater in magnitude than that due to mechanical compaction of the pore space.

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