



Nuclear Magnetic Resonance Permeability Models by Partial Least Square Regression

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Abstract

This study explores the application of Partial Least Squares Regression (PLSR) in modeling rock permeability from Nuclear Magnetic Resonance (NMR) relaxation data. The ¹H transversal relaxation T₂ curves of 68 sandstone core plugs from outcrop analogues and Brazilian reservoirs, with permeability ranging from 0.007 to 9,800 mD and fully saturated with saline solution, were measured at 2MHz. The T₂ spectra were obtained by inverse Laplace transformation (ILT) and permeability was firstly estimated with the classical Timur Coates and Schlumberger-Doll Research models. The resulting prediction curves presented a non homogeneous response along the calibration interval and a root mean square error (RMSE) of 0.70 log mD for both models. In the other hand, the PLSR models, based on the T₂ relaxation spectra (inverted data) and also on the relaxation curves (raw data), presented a more homogeneous and accurate response, computing a RMSE of 0.47 and 0.50 log mD, respectively.

Introduction

The knowledge of permeability and porosity of rock formations is a key step in the exploration of natural resources like groundwater and petroleum. While the porosity represents the reservoir storage capacity, the permeability responds for its deliverability. These important petrophysical parameters can be indirectly measured by geophysical methods based on the principle of Nuclear Magnetic Resonance (NMR), the only technique sensitive to pore-size distribution, pore structure and permeability (Kenyon, 1997; Prammer, 2004). While in oil exploration the NMR measurements are performed down hole using well-logging tools that generate their own magnetic field (Jackson, 2001), in hydrogeology, the NMR technique, known as proton Magnetic Resonance Sounding (MRS) is performed at the earth's surface using the natural geomagnetic field (Yaramanci et al., 2008).

When submitted to a static magnetic field (B₀) the NMR active nuclei, like ¹H present in molecular composition of reservoir fluids (water, oil or gas), buildup a resultant nuclear magnetization (M₀) aligned to the B₀ direction. The characteristic time constant for this

exponential phenomenon is denoted as T₁ (longitudinal relaxation time). After disturbing the magnetization with a radio frequency pulse (B₁), it returns to the initial state, in a process called nuclear magnetic relaxation. During the relaxation, M₀ induces an electrical current in a detection coil, the NMR signal or Free Induction Decay (FID), which decays exponentially with a characteristic time constant denoted T₂ (transversal relaxation time). The initial amplitude of the FID is given by M₀, which is directly proportional to the amount of fluid present in the rock formation. Assuming a relaxation regime where the rate-limiting step is relaxation at the surface, denoted fast diffusion regime (Brownstein and Tarr, 1979), either the M₀ buildup or the NMR signal decay rate will depend mainly on the surface-to-volume ratio of the pore:

$$\frac{1}{T_{1,2}} = \rho_{1,2} \left[\frac{S}{V} \right]_{\text{pore}}, \quad (1)$$

where ρ₁ and ρ₂ are the surface relaxivity for T₁ and T₂, respectively, which is a measurement of the pore surface ability to enhance the relaxation rate.

According to the Eq. 1, the saturating fluid relaxation times will vary according to the porous radius; small pores have small T_{1,2} values and large pores have large T_{1,2}. For a natural porous media, like sedimentary rocks, which usually exhibits a pore size distribution, the ¹H NMR signal decay (and also the build-up curve for T₁) can be modeled as a linear combination of characteristics relaxation times of each pore size saturating fluid (Watson and Chang, 1997). For a single fluid, like water, each point of the T₂ relaxation curve, for example, can be generically written as:

$$I(t_j) = \sum_k A(T_{2,k}) \exp(-t_j / T_{2,k}) + \varepsilon_j, \quad (2)$$

where I(t_j) is the NMR signal amplitude at a time t_j; A(T_{2,k}) is a distribution function of the transverse relaxation time T₂ for fluid occupying the k-sized pore; and ε_j is the noise.

The typical approach adopted by the NMR data interpreters is to calculate the relaxation time distribution functions A(T_{2,k}), also known as relaxation spectra (Provencher, 1982), using inverse Laplace transformation (ILT). The relaxation spectra provide the basis of the most important permeability estimation models used in the oil exploration activity: the Timur-Coates, TC model (Coates et al., 1991), and the Schlumberger-Doll Research, SDR model (Kenyon et al, 1986). However, it is well known that the ill-posed nature of the Laplace inversion, where the solution is not unique and/or has a critical dependence with the input data, has potential to produce unrealistic peaks in the relaxation spectra. Although the Laplace inversion algorithms incorporate regularization schemes

to stabilize the final solution inversions, like Tikhonov regularization (Tikhonov et al., 1977) and maximum entropy method (Skilling, 1989) it is still difficult to determine the reliability and error of the resulting distributions.

Recently, Ramos et al. (2009) demonstrated the successful application of Partial Least Squares Regression (PLSR) in modeling crude oil viscosity from T_2 spectra and directly from raw relaxation curves. PLSR is a multivariate data analysis (MVA) method particularly well suited to deal with ill-posed and multicollinear problems, such as those frequently encountered when modeling from NMR data. The underlying assumption of a PLSR model is that the system of interest is driven by a few orthogonal latent variables (LV=a), which are linear combinations of observed explanatory variables. Suppose we have two matrices, the predictors variables $X_{n \times k}$ (e.g. NMR spectra bins) and the responses variables $Y_{n \times m}$ (e.g. rock petrophysical properties), where the columns correspond to variables and the rows to observations. The PLSR decomposes these matrices into the form:

$$X_{n \times k} = T_{n \times a} P_{a \times k}^T + E_{n \times k}, \quad (3)$$

$$\text{and } Y_{n \times m} = U_{n \times a} Q_{a \times m}^T + F_{n \times m}, \quad (4)$$

where the $T_{n \times a}$ and $U_{n \times a}$ are matrices of scores, sample projections on the new latent variables directions; $P_{a \times k}$ and $Q_{a \times m}$ are matrices of loadings, cosines of angles between the latent variables and the original variables directions and; $E_{n \times k}$ and $F_{n \times m}$ are matrices of non-explained variance, or residuals.

PLSR algorithms choose iteratively successive orthogonal latent variables that maximize the cross-covariance between X and Y variables, producing scores values that both well summarize the variance of predictors and highly correlate with response variables. The original predictors and response variables are replaced by these new reduced set of latent variables, so that a regression model is set up between their scores. See Chatfield and Collins (1980), and Harald and Naes, (1989), for a more detailed explanation of PLSR methods.

Our purpose in the present work is to explore the benefits of the multivariate data calibration techniques like PLSR to develop regression models for permeability estimation based either on the T_2 relaxation spectra or on the T_2 raw decays (without the need of inverting the relaxation curves). The developed models are expected to predict the log of permeability of sedimentary rock samples over seven degrees of magnitude scale better than the classical TC and SDR models.

Method

For this study, 68 consolidated sandstone cylindrical plugs (3.81 cm x 5.00 cm) from outcrop analogues and Brazilian reservoirs with a wide range of permeability (0.007 to 9,800mD) and porosity (3.4% to 33.6%) were selected. The samples were cleaned by successive extraction cycles with toluene (for hydrocarbons removal) and methanol (for water and salts removal), according to the recommended practices of the American Petroleum Institute (API, 1998). The routine porosity (ϕ) and absolute permeability (K) were measured at 500PSI at 25°C in an

UltraPore 300 and Ultraperm 500 (both from Core Lab, USA), respectively. After these routine core analyses, the samples were saturated with a 50,000ppm NaCl solution of by vacuum followed by pressure of 2,000PSI.

Transversal relaxation time measurements, T_2 , were performed in duplicate at 35°C in a 460 Gauss (2MHz for ^1H) bench-top NMR spectrometer Maran Ultra (Oxford Instruments, UK), using a 52mm probe. The T_2 measurements were performed using the Carr-Purcell-Meiboom-Gill (Meiboom and Gill, 1958) pulse sequence with time between echoes of 200 μs , 32 scans, 8192 echoes and recycle delay of 10s.

The T_2 relaxation spectra were processed with 128 points logarithmically distributed between 0.1ms and 10s. The ILT was performed using the 2D Laplace Inversion ver.2 (Magritek, New Zealand) software. Before the PLSR modeling, all the spectra were normalized to the unit area and mean-centered. Due to a broad and skewed distribution in the permeability values they were also log-transformed. The PLSR model was fully-cross validated using the leave-one-out scheme (Efron and Tibshirani, 1993). The MVA modeling was performed by the The Unscrambler ver.9.8 (Camo, Norway).

Results

Fig.1 shows the T_2 ^1H relaxation curves for the free saline solution (bulk relaxation) and for three fully saturated sandstone plugs with different poroperm properties. As can be observed, the rock matrix surface acts like a relaxation sink and the relaxation curve decays more rapidly when the fluid is confined into the pore space. While the NMR signal for the solution remains detectable for more than 3 seconds, for plug P-53 it is gone at about 200 milliseconds.

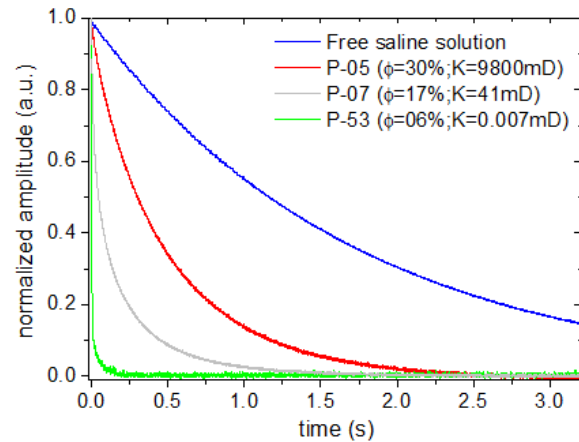


Figure 1 – NMR T_2 decaying signal (normalized by maximum amplitude) for the free saline solution and three saturated core plugs: P-05, P-07 e P-53. The plug porosities and permeabilities are indicated.

For the free saline solution, where all water molecules are indistinguishable, it was possible to fit its relaxation curve with a monoexponential decay function and to extract a discrete T_2 relaxation time. However, when the solution is filling the rock pore space, surface relaxation mechanisms also modulate its NMR signal producing a multiexponential decay that will vary according to the pore

size distribution (Dunn et al., 2002), thus the recommended approach in this case is to process the relaxation curves by means of ILT.

Fig. 2 shows the relaxation spectra, normalized by unit area, inverted from Fig.1 raw curves by ILT. While the saline solution presents a singular T_2 value about 1.8s, the saturated plugs spectra have T_2 values shorter than it and usually spreading over more than one logarithmic cycle according to the pore size distribution. Computing the area under these spectra, it is possible to classify different types of water according to the relaxation time range. For sandstones, $T_2 < 3ms$ correspond to the clay bond water (CBW) and $3ms < T_2 < 33ms$ is the capillary bound water (Coates et al., 2001). These two types of water account for the Bulk Volume Irreducible (BVI). Above a 33ms $T_{2cut-off}$ (sandstones), it is possible to find the drainable or free water. Its related area under the spectra is called Free Fluid Index (FFI).

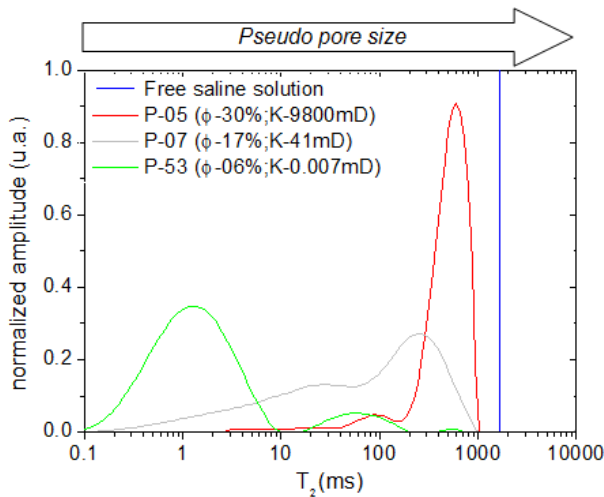


Figure 2 – NMR T_2 relaxation spectra or pseudo pore size distributions. The vertical line corresponds to the discrete T_2 value for the free saline solution, about 1.7s.

Once the initial amplitude of the decaying NMR signal (I) or the total area under the spectra (A) depends directly from the amount of fluid present in the pore space, comparing it to the signal amplitude of a standard sample or a known volume (V) from the bulk saline solution, it is possible to indirectly measure the rock porosity (Coates et al., 2001). The plug porosities were calculated from the following form:

$$\phi_{NMR} = \left(\frac{V}{I}\right)_{SOL} \times \left(\frac{I}{V}\right)_{PLUG} = \left(\frac{V}{A}\right)_{SOL} \times \left(\frac{A}{V}\right)_{PLUG}, \quad (5)$$

where $(V/I)_{sol}$ and $(V/A)_{sol}$ are the calibrating factor measured with the bulk solution for the raw and inverted T_2 relaxation data, respectively.

Fig.3 shows the excellent agreement observed between routine porosity, directly measured with the conventional gas porosimetry, and porosity derived from NMR measurements of the fully saturated samples, applying Eq. 5. For the great majority of the samples it was possible to predict porosity with an accuracy of almost 1 porosity unity (p.u.). The cross-plot of Fig.3 is

also useful for quality control, the excellent agreement between the two porosities ensures that the NMR results are reliable and the samples are well characterized and prepared.

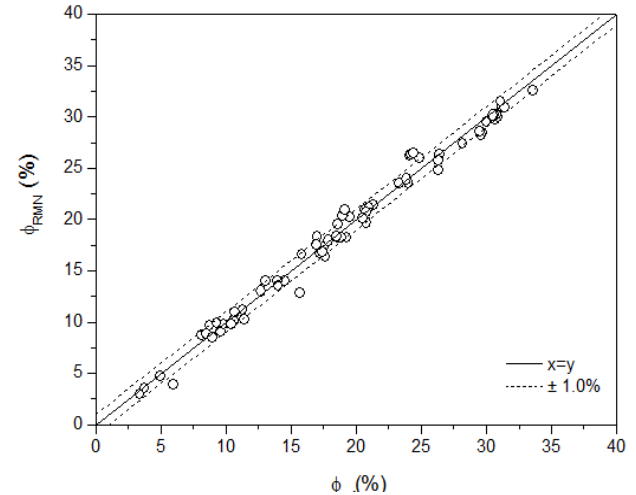


Figure 3 – Routine core analysis porosity (ϕ) against NMR predicted porosity (ϕ_{NMR}).

It is well known that permeability K (mD) is governed by pore connectivity (i.e. pore throats), rather than pore size, and what most empirical correlations do is to rely on a correlation between pore sizes and pore throats to predict permeability from NMR data (Fleury et al., 2001). The TC and SDR models, the two most spread in the petroleum industry, are based on the fact that pore size is relatively proportional to pore throat, assumption valid mainly for siliciclastics. They respectively adopt the FFI/BVI ratio and the spectra geometric mean (T_{2gm}) as a representation of the average pore size, besides porosity ϕ (%), to predict the permeability, as indicated in the following equations:

$$K_{TC} = a \left(\frac{FFI}{BVI}\right)^b \phi_{NMR}^c, \quad (6)$$

$$\text{and} \quad K_{SDR} = a T_{2gm}^b \phi_{NMR}^c, \quad (7)$$

where 'a', 'b' and 'c' are empirical coefficients.

From the experimental measured T_2 spectra the coefficients of both models equation were adjusted to match the 68 plugs absolute permeability by a multiple linear regression (MLR). The FFI/BVI ratio was calculated considering a 33ms $T_{2cut-off}$ for standard sandstones. Tab.1 shows the TC and SDR models optimized coefficients.

Table 1 – Empirical TC and SDR models coefficients.

Model	Empirical Coefficients		
	a	b	c
TC	4.47×10^{-3}	1.70	2.30
SDR	4.6×10^{-12}	1.98	2.49

Fig. 4 presents the response curve for the TC (Fig.4a) and the SDR (Fig.4b) classical NMR permeability models with the previous calculated coefficients. In both curves it is possible to observe a lack of predictability for samples with routine absolute permeabilities less than 1mD. Both models computed a RMSE of 0,7 log mD.

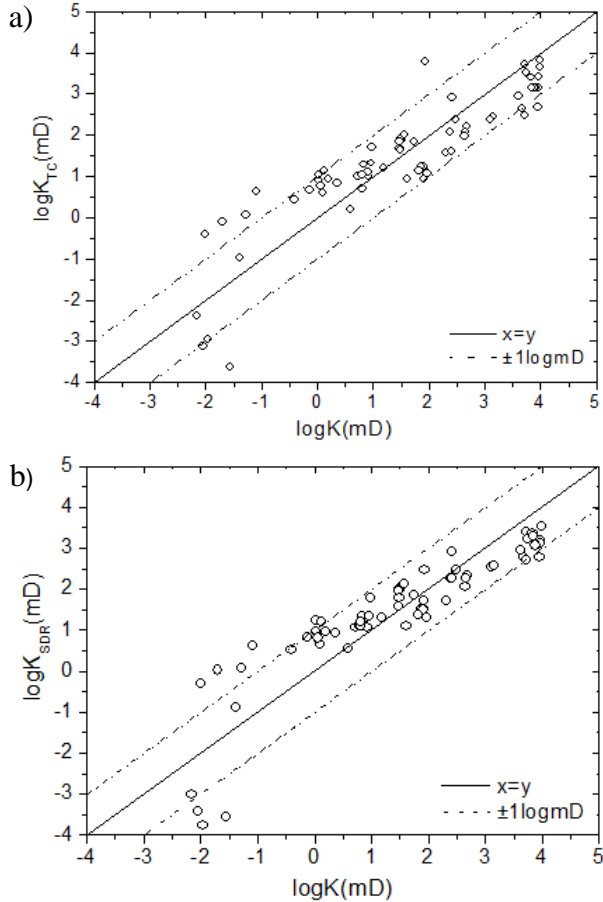


Figura 4 - a) TC and B) SDR permeability estimations compared to routine absolute permeability.

Classifying the samples into two groups: G-A for $K > 1\text{mD}$ and G-B for $K \leq 1\text{mD}$, different poroperm trends can be identified in the permeability porosity cross plot, Fig. 5. Besides, these groups have different percentage of Clay Bound Water porosity (CBW) with G-A $< 20\%$ e G-B $\geq 20\%$, quantified with a T_2 Clay Bound Water Cut off ($T_{2\text{CBW}}$) of 3ms in the relaxation spectra (Coates et al., 2001).

This fact suggest that microporosity associated with clays could be one of the reasons of the low performance of the classical models in predicting a wide range of permeability values, more than six cycles in the logarithmic scale. Although this microporosity do not contribute to the fluid flow at the same extension when compared to the intergranular porosity, it shifts both the FFI/BVI and the $T_{2\text{gm}}$ down (small values). In this sense, it is justified that samples with higher CBW values have permeabilities values much less than expected, when compared to other samples with the same porosity but with reduced CBW percentage.

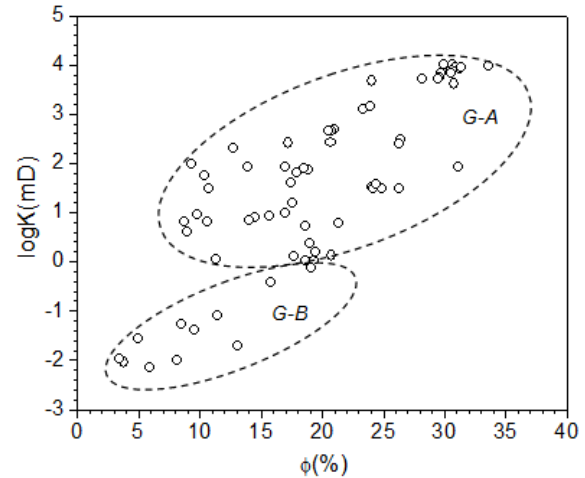


Figure 5 - Routine porosity (ϕ) versus absolute permeability (K). Samples arbitrarily grouped as G-A ($K > 1\text{mD}$, $\text{CBW} < 20\%$) and G-B ($K \leq 1\text{mD}$, $\text{CBW} \geq 20\%$).

To evaluate the application of PLS regression in permeability estimation two models were constructed from the predictors matrixes: $X_{68,129}$, containing the NMR porosity and the respective T_2 spectra (inverted data); and $X_{68,8183}$, containing the NMR porosity and the T_2 relaxation curves (raw data). They were calibrated with a $Y_{68,1}$ response matrix, containing the plugs routine absolute permeabilities. The equation for both models can be expressed, respectively, as following:

$$\log K_{\text{PLS}} = b_0 + b_1\phi + \sum_{k=1}^{128} b_{k+1}A(T_{2,k}) \quad (8)$$

$$\log K_{\text{PLS}} = b_0 + b_1\phi + \sum_{j=1}^{8192} b_{j+1}I(t_j) \quad (9)$$

where b_0 is the coefficient for the intercepts and the other b 's are the PLS regression coefficients for the predictor variables (porosity, the 128 T_2 inverted data bins and the 8192 raw data bins).

Fig.6a shows the RMSE for the PLSR spectra based models with different latent variables (LV) compared to the computed classical models RMSE (0.7 log mD). Fig.6b is the response curve for the chosen 6 LV model (optimized to achieve a parsimonious compromise between model stability and accuracy). It presented a Y-explained variance of 94% and a RMSE of 0.47 log mD. Fig.6c presents the respective regression coefficients with a clear bipolar behavior. Positive values at T_2 above 170ms, indicate the direct relationship between larger pore sizes and permeability, and negative coefficients at T_2 lower than 170ms, indicate an inverse relationship with the smaller pores.

The PLSR algorithm performed better than the classical models, presenting a more homogeneous response over the entire calibration interval. This superior response can be attributed to the multivariate nature of this regression, where each relaxation point of the T_2 spectra (related to a pore size family) is weighted by its own regression coefficient, based on its particular contribution to the permeability estimation. In the classical models all the variability present on the relaxation spectra

is simply summarized by a singular mean T_2 relaxation time: $T_{2cut-off}$ (TC) and T_{2gm} (SDR). Those models do not take account that each pore size may have a particular and complex correlation with pore throat and consequently to the permeability.

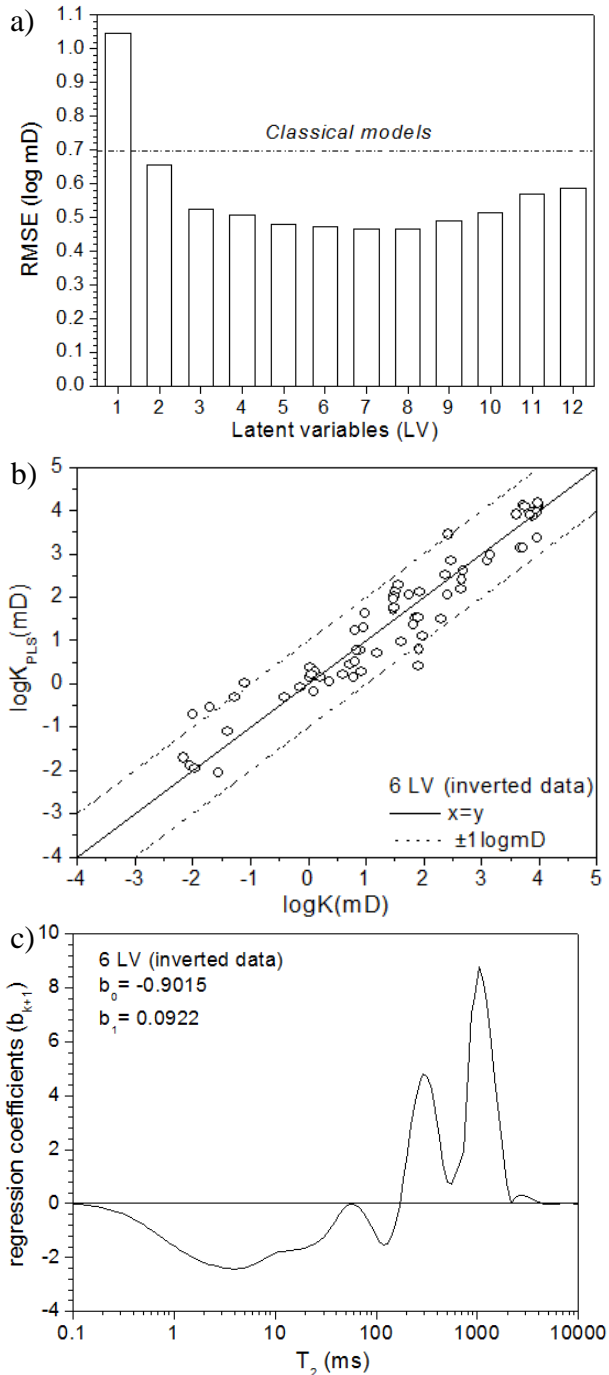


Figure 6 – a) RMSE of different Latent Variables PLSR model from inverted relation data compared to the classical models RMSE obtained. b) Response curve for the 6 LV chosen PLSR model and its, c) respective regression coefficients curve.

Fig.7a shows the RMSE for the PLSR raw data based models with different numbers of Latent variables; Fig. 7b the response curve for the chosen 2 LV model, with a Y-explained variance of 92% and a RMSE of 0.47 log mD; and Fig.7c its regression coefficients, not directly interpreted because of its time domain representation.

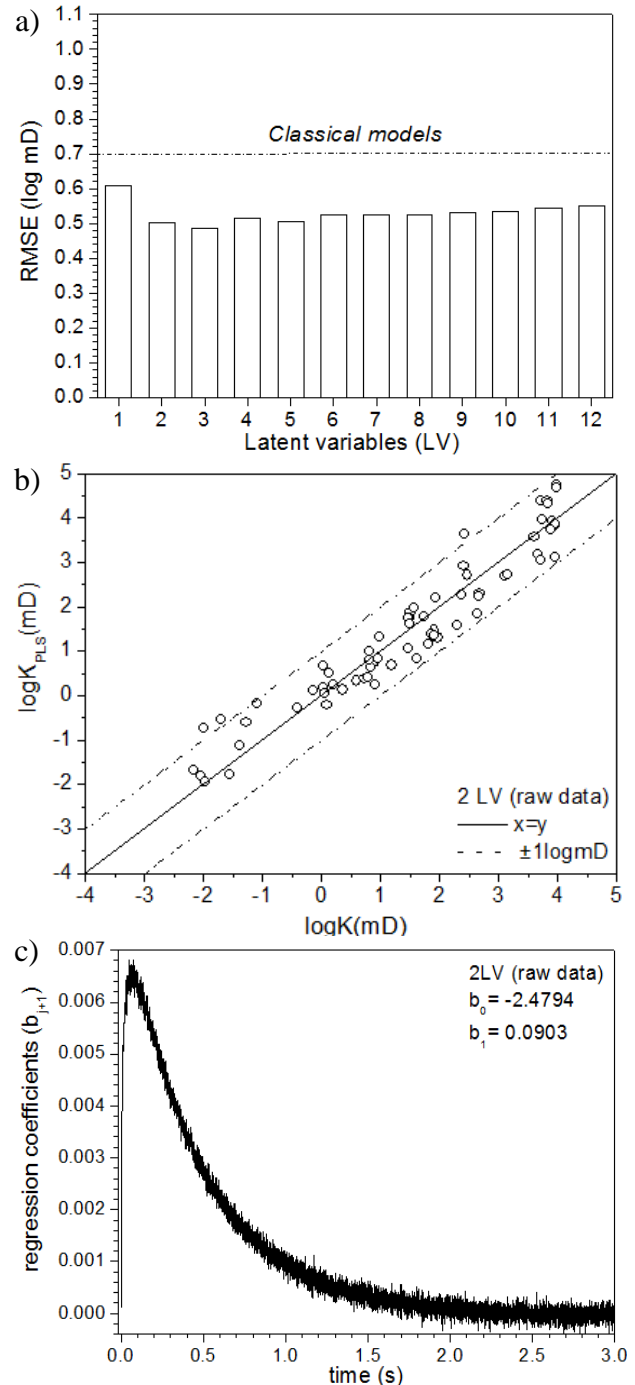


Figure 7 – a) RMSE of different Latent Variables PLSR model from raw relation data compared to the classical models RMSE obtained. b) Response curve for the 2 LV chosen PLSR model and its, c) respective regression coefficients curve.

The raw T_2 data based PLSR model performed slightly better, regarding its accuracy, when compared with its analogue developed for relaxation spectra. This result is a very significant achievement, because the inverse Laplace transformation, as mentioned before, can potentially generate spurious responses on the relaxation spectra (Provencher, 1982), mainly considering that NMR data is frequently acquired with low signal/noise ratios.

Conclusions

We demonstrated that PLSR technique can model rock permeability, in log mD units, over a broad range of values, almost 7 orders of magnitude. The superior accuracy and more uniform response presented by the PLSR models, when compared to the classical TC and SDR models, suggest that the multivariate modeling approach is more appropriate than the 'average singular pore size' classical ones, even when different poroperm trends take place in the analyzed data set. Analog performances are solely achieved by other models in the literature when coefficients are optimized for each individual formation rock type; applying permeability range segmentation; or even including resistivity measurements.

Additionally, it was also demonstrated that NMR permeability models based on PLSR can also be built directly from the raw relaxation curves, with quite similar characteristics of those developed with the relaxation spectra. This result is particularly important, once the common practice among the NMR well logging interpreters is to work exclusively with the inverted relaxation data, which depends on regularization schemes to stabilize the distribution functions. This is an extremely relevant feature, mainly considering that inversion of noisy NMR data is recognized as an inherently non-unique process.

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