Discrete Inversion NMR (DI-NMR): An NMR data processing method for Accurate Fluid Typing and Saturation Determination

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Abstract. Accurate fluid typing and quantitative saturation determination are essential to evaluate reservoir production potential, which is a well-accepted deliverable of NMR technology. However, challenges remain in obtaining these critical reservoir properties due to the ill-posed nature of conventional Inverse Laplace Transform (ILT)-based NMR data processing method and partitioning of overlapping continuous NMR relaxation time distributions from both 1D and 2D data. This work presents a solution for these problems since the inception of low-field NMR in the O&G industry over 60 years ago. The first step in existing NMR data processing and interpretation is to convert raw time decay data by the ILT inversion with the known issue of overlapping peaks with similar relaxation times. Partitioning the overlapping peaks for fluid typing is usually performed using manual cut-off, Gaussian decomposition, or machine learning methods, with considerable uncertainty and inconsistency. The discrete inversion method generates a unique number of discrete components with the accurate quantity directly corresponding to the specific fluid type from the NMR raw data, time domain NMR signal decay curve. The proposed DI-NMR, a conventional ILT, and an improved ILT method are applied to 1D and 2D measurements on synthetic samples, bulk fluid mixture (brine and filtrate), and shale samples for comparison. For the synthetic samples of individual components, the DI-NMR method returned the components of accurate amplitudes and NMR relaxation times. In contrast, the ILT methods only provided estimated amplitudes and relaxation times through manual partitioning. The DI-NMR results from mixed bulk fluids also agreed very well with those from separate measurements. The true potential of the new workflow was illustrated in the analysis of shale samples, where different fluid types, such as free oil, free water, absorbed oil, and clay-bound water, were easily determined and quantified by directly assigning the discrete components based on their NMR relaxation time values according to a general fluid typing NMR scheme. The successful ongoing testing on the conventional T2 logging data of low signal-to-noise ratio indicates that it works well for logging as well. In summary, accurate and robust fluid typing and saturation determination could be achieved by using the DI-NMR method, which eliminates the uncertainty, ambiguity, and inconsistency of ILT-based two-step approaches.

1 Introduction

Nuclear magnetic resonance (NMR) is considered one of the important technologies to determine rock formations' petrophysical properties and probe the formation fluid types and saturation. Since its wide application in the 1990s, it has continuously developed and improved in all aspects to meet various needs. One recent example is its success in tackling unconventional reservoir characterization, where many other commonly used technologies developed for conventional reservoirs do not work well (1). Specifically, the fluid typing and quantification for shale can be achieved from the 2D NMR T1-T2 data through NMR data post-processing techniques such as manual cut-off, curve fitting, and machine learning methods (2, 3, 4).

The current work proposes a new fluid typing and quantification approach based on a discrete inversion technique called the Anahess method (5, 6). For quantitative post-processing after inversion including fluid classification and quantification, it provides a more accurate and efficient workflow, skipping the partitioning of overlapping distributions by the ILT inversion method. In fact, the continuity of 2D distributions from different fluid components is partially imposed by the ILT methods itself. Unlike the ILT, the discrete inversion methods offer straightforward user-independent fluid typing and quantification. Anahess method is one of the inversion methods introduced for NMR data processing to obtain discrete or sparse distributions different from continuous distributions by the ILT methods. Reci et al. (7) obtained sparse distribution for increasing spectral resolution, while Yarman and Mitchell (8) recently obtained discrete solutions for downhole limited data bandwidths. The Anahess method first provided a robust alternative to the ILT methods (5) and subsequently combined with ILT (6) to generate both discrete and continuous solutions for quantitative and qualitative applications. These discrete and sparse inversion methods are expected to find more quantitative petrophysical applications in other NMR measurements for the right situations, just as the ILT methods. In this work, we present a set of results using the DI method to process T2, 2D T2-D, and 2D T1-T2

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data. A brief review of existing shale fluid typing /quantification methods and NMR inversion methods, including both ILT and DI methods, is first presented to explain the background and motivation of the current development.

1.1 Shale fluid typing and quantification from T1-T2 maps by the ILT methods

Accurate quantification of fluids in the shale poses a significant challenge because of the ~nm scale pore size, pore types, and complex fluid types such as free oil/water, hydroxyls, kerogen, etc. Nuclear magnetic resonance shows its unique strength due to its high sensitivity to protons in all types of fluids. It has gained wide applications in the O&G industry, including shale formation evaluation (9). Specifically, 2D T1-T2 has been applied successfully for fluid characterization in shale. Since the publication of Fleury et al. (2), a series of 2D NMR data interpretation schemes have been proposed for shale samples from different target regions and in various states. Mukhametdinova et al. (10) reviewed and summarized the eight most widespread data interpretation schemes and proposed a universal one with six essential regions or fluid types based on the best fitting of interpretation results to laboratory data. Each fluid is found to correspond to a specific area on the T1-T2 maps defined by approximate T1, T2, and T1/T2 ratios, from which its volume is determined from the total amplitude over the area.

Even though all fluids presented in the sample can be detected by 2D T1-T2, simple regional cut-off methods do not appear to be efficient and accurate for accurate fluid typing and quantification. A series of sophisticated methods are developed to automatically perform fluid typing and quantification. One of them is based on the Gaussian decomposition, similar to the 1D T2 Gaussian decomposition (3,11). Some of the recent methods take advantage of data-driven clustering techniques. Jiang et al. (12) compared the performance of six common clustering algorithms for characterizing fluids in the shale from 2D NMR data and claimed the Gaussian mixture model (GMM) performed the best. Venkataramanan et al. (4) developed a method utilizing an automated unsupervised learning algorithm called blind-source separation (BSS) for quantifying the volumes of different fluid components from 2D T1-T2 well logging data. All of the above methods are based on 2D T1-T2 data processed by the ILT methods, which unavoidably contain additional constraints such as the regularization (smoothing) factor; however, their effect on the partitioning and accuracy was not studied in detail.

1.2 Inversion methods

NMR relaxation is modeled by a Fredholm integral equation of the first kind, and the ill-posed nature of the inversion problem means that an entire ensemble of infinite solutions exists. The ILT methods with Tikhonov regularization are the most commonly used methods of NMR data processing, while other methods are proposed (13, 14, 15). Mitchell et al. (16) reviewed the ILT methods and summarized three sets of general constraints on the resultant distributions: non-negative, range/spacing of the distribution, and smoothness bias. The following sections discuss the regularization and spectral resolution of the ILT methods and review the sparse and discrete methods, which are explored for applications in shale fluid typing and quantification.

1.2.1 Smoothness, spectral resolution, and uncertainty of the ILT methods

The ILT methods successfully generate continuous and stable NMR relaxation time distributions with noise generated from the measurements. They are considered as the actual continuous pore size distributions and crude oil distributions, which are successfully applied for the NMR data interpretation. However, the degree of applied regularization factors, which are directly related to spectral resolution, and their effect on fluid typing and quantification should be evaluated. The regularization factor is determined by the trade-off of data fitting quality and model complexity. The spectral resolution of Tikhonov regularization is low, and features with relaxation time differences from each other by a factor of ~3 or less cannot be distinguished (7). The signal-to-noise ratio (SNR) also plays a role in the smoothness of the continuous distributions. Song et al. (15,17) indicated that the resolutions of inverted 1D T2 distribution match the actual resolutions when SNR is above around 100 and higher. The actual spectral resolutions may not be restored at lower SNR. The SNR of 2D T1-T2 data is relatively low compared to that of 1D, especially for well-logging data, mainly due to the longer data acquisition time requirement. Thus, the fine features sharper than the unknown smoothness imposed by ILT cannot be inverted fully. Furthermore, the smoothness appears to change with relaxation times. With the synthetic 2D T1-T2 data examples presented in the later section (Fig. 1), it is speculated that the final T1-T2 maps are the result of the data with different smoothness at different times, which is not fully considered in the ILT-based partitioning methods. There could be other uncertainties regarding the ILT methods, such as artifacts, which have not been fully studied in the literature. Some uncertainties of the ILT methods are only illustrated by comparison with other inversion methods (e.g., sparse and discrete) instead of complex numerical analysis of the ILT methods themselves, as shown in later examples (Fig. 1).

1.2.2 Sparse and discrete inversion methods

Some solutions in the entire ensemble of infinite solutions from the inversion problem could take completely different forms from the continuous solutions by the ILT methods. Prange and Song (18) used boxcar functions to investigate the T2 spectral uncertainty. In fact, solutions with different Smoothness can also be obtained from the ILT methods by adjusting the regularization factor. Just as the ILT methods, sparse and discrete methods also impose constraints on their solutions and are not claimed to be closer to the actual distributions. They are investigated for potentially more straightforward subsequent partitioning analysis for shale fluid typing and quantification.

Reci et al. (3) used the L1 form instead of the L2 form in regularization to obtain sparse distributions. Features with relaxation time differences of as little as 10% can be distinguished compared to a factor of 3 using L2 form regularization. Hexane and dodecane in bulk liquid mixtures and in porous media can be well separated. Similar to the potentially excessive broadening of L2 form regularization, in the opposite way, L1 regularization tends to break actual wide continuous peaks into a cluster of narrow peaks. Combinations of L1 and L2 norms are proposed by other researchers (19) to reduce constraints on the solutions.

Ukkelberg and Sorland (5) developed the Anahess method using discrete components, and Yarman and Mitchell (8) developed a greedy variational method for discrete inversion utilizing a sum of Dirac functions. It is strikingly surprising that not too many components are needed for both methods to obtain a similar fit quality as other ILT methods. Four to nine components could usually be sufficient to fit the data well for rock samples by the Anahess method (5). On synthetic data sets, Yarman and Mitchell's method returns all or fewer components with more significant noise levels; on rock sample data sets, the components agree with the smooth peak maxima of distribution from the Tikhonov method, and their amplitudes are equal to the sum of the corresponding peaks. Both Anahess and greedy variational methods are considerably insensitive to noise. It is worth noting that fitting residual distribution might be another indicator of fitting quality in addition to levels of fitting residual. The fitting residual distribution should be Gaussian if the instrument is free of systematic errors. Both the Anahess and greedy variational methods have Gaussian-shaped fitting residuals, while the ILT methods may not (6, 8).

The Anahess method was first developed as a pure discrete method and was later combined with ILT, providing continuous distributions reflecting the actual ones. With a known number of components, it is much simpler and more robust to interpret the 2D T1-T2 data for the further analysis of fluid typing and quantification, especially when the ILT method generates an overly continuous map without clear features. The known number of components determined by discrete inversion can also help the ILT methods produce data reflecting the actual system by grouping the discrete components and adjusting the broadening factor. The Anahess method provides a complete solution of both discrete components for subsequent quantification and continuous distributions for better understanding, while other sparse and discrete methods usually focus on discrete solutions only. The following section discusses the discrete method used in this report, Anahess, with more details.

1.2.3 Anahess discrete inversion

The Anahess method is designed to find a unique number of discrete exponential components according to the fitting stop criteria to fit the raw experimental relaxation data (5,6). It was named after the terms ("Analytical expression" and "Hessian matrix" (6)) in the procedure, which is used by the optimization algorithm. The function to be minimized from 2D T1-T2 data takes a similar form to the ILT except for the missing regularization term and different arbitrary relaxation times from the logarithmically equal spaced times of the ILT:

$$SS_{res}F(a_0, a, T_1, T_2) = \sum_i^{NSA} \sum_j^{NSE} \left\{ f(a_0, a, T_1, T_2) - R_{i,j} \right\}^2 \qquad (1)$$

where

$$f(a_0, a, T_1, T_2)_{i,j} = a_0 + \sum_p^{NCO} a_p e^{1-\left(\frac{1}{T_{1,p}}\right)g_i - \left(\frac{1}{T_{2,p}}\right)t_j}$$

$$a_p, T_{1,p}, T_{2,p} \geq 0, and\ p = 1 \ldots NCO \qquad (2)$$

The component parameters, a_p, $T_{1,p}$, $T_{2,p}$, are all larger than or equal to zero, $R_{i,j}$ is the experimental measurement, and NSA and NSE are the numbers of rows and columns of the experimental data. NCO is the number of components. Further details of the solving algorithm (inverse Hessian matrix, univariate minimization, choice of the initial estimate, and the number of components) can be found in Ukkelberg et al. and Sørland et al.'s work (5, 6). In the current work, synthetic data sets are processed by this method again to compare with the ILT methods.

The Anahess method has been further combined with the ILT to take advantage of both methods to produce Anahess/ILT continuous distributions without most of the constraints of common ILT methods (20). Extensive comparison of the results of sparse and discrete methods could be another interesting topic.

2 Experimental samples and procedures

The proposed Anahess-based DI-NMR method is robust and accurate compared to the ILT methods without the need for complex subsequent partitioning continuous 1D and 2D distributions for quantification. The new DI-NMR workflow has been tested on a set of NMR data and produced promising results for fluid typing and quantification. Two types of data, a synthetic and a bulk fluid mixture, are presented to illustrate the differences between the methods, and a shale sample data is presented to demonstrate the new workflow.

The details of the synthetic data set can be found in Althaus et al.'s paper (21). 10% noise is added to the synthetic signal. The volume, T1, and T2 of the peaks are listed in Table 1. The bulk fluid mixture is composed of 5 ml of high salinity formation brine and 5 ml of oil-based mud (OBM) filtrate in a 20 ml glass vial. Finally, the preserved shale sample has been used for the current study.

The T2, T1-T2, and T2-D measurements of the bulk fluid mixture were conducted using a 2 MHz NMR instrument, with an echo delay (TE) of 200µs. The signal-to-noise ratios (SNR) of T2, T1-T2, and T2-D are 133, 85, and 38, respectively. The T1-T2 data of the shale sample was acquired by a 12 MHz NMR instrument with TE = 55µs.

The data are processed using two versions of ILT, called ILT1 and ILT2 here, and the proposed DI-NMR method. ILT1 is commonly used in the industry, and its regularization factor is automatically selected based on the SNR of the raw data. ILT2 is an improved version of the ILT method with the regularization parameters computed by the automatic update rule (22). It is worth mentioning that the objective of this practice is not to rate different inversion methods but to explore the potential of the new DI-NMR method for accurate fluid typing and saturation determination.

3 Results and discussion

The results of data analysis for three groups of samples are reported below. Currently, the new workflow is demonstrated by simply applying a general fluid typing scheme of discrete components of laboratory core samples on the 3D bubble graph for identification and quantification.

3.1 Synthetic sample

The synthetic data set has three peaks with their volumes and relaxation times (T1 and T2) listed in Table 1 and Table 2 as input. The relaxation time of peak 1 is the shortest, peak 3 is the longest, while peak 2 is between peak 1 and peak 3. The peaks have similar relaxation times of typical shale samples.

Table 1. Peak volumes calculated by different data processing techniques for the synthetic sample.

Data	Volume (ml)			
	Peak 1	Peak 2	Peak 3	Total
Input	1.9	1.4	2.9	6.2
ILT-1	2.1	1.4	2.9	6.9
ILT-2	2	1.5	2.8	6.6
DI-NMR	1.9	1.4	2.9	6.2

Table 2. Relaxation times of the synthetic sample from DI method.

Components	T1 (msec)		T2 (msec)	
	Input	DI-NMR	Input	DI-NMR
Peak 1	5	4.906	0.2	0.1968
Peak 2	200	201.7	0.2	0.2003
Peak 3	100	99.9	10	9.99

3.1.1 T1-T2 distributions

The 2D T1-T2 distributions generated by ILT1, ILT2, Anahess, and Anahess/ILT of the synthetic sample are presented in Figure 1. Unlike ILT, the Anahess method only produces the amplitude and relaxation times of discrete components. They are plotted using a 3D bubble graph to show the locations and relative amplitudes of the components, not the distributions. The differences in NMR peaks generated by four different methods are obvious. The additional spurious peaks and the broadening of the short relaxation peaks from both ILT methods are similar to other works on synthetic data reviewed in the previous section. The challenges are expected for subsequent partition methods on actual data with closer or overlapping peaks, even for the ILT2 method. On the contrary, the Anahess method returns almost exact volumes considering the added noise. The larger total integral volume of the ILT methods in Table 1 may indicate small distributions not covered by three peak areas, such as baseline, edge effect, etc. In addition, the relaxation times are returned accurately by the Anahess method (Table 2), while they can be approximately calculated within the peak areas weighed by amplitudes for the ILT methods.

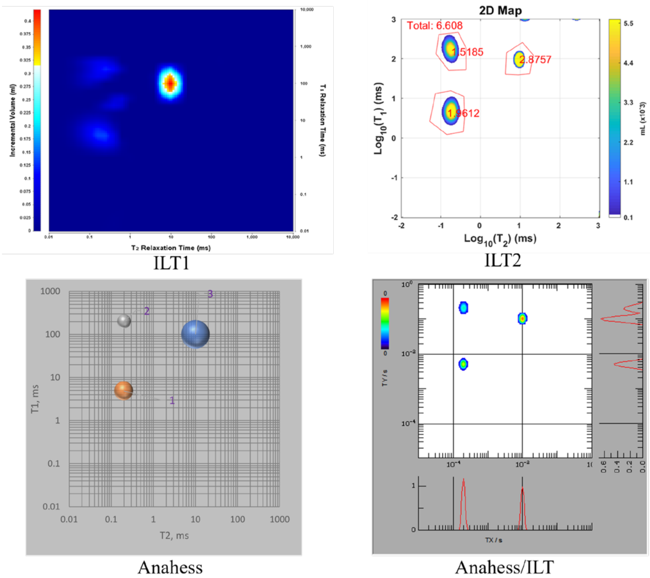


Fig. 1. 2D T1-T2 distributions of the synthetic sample.

3.2 The mixture of bulk fluids

A suite of NMR data, T2, T1-T2, and T2-D, are also acquired for a fluid mixture with known distributions, 5ml of brine and 5 mil of oil-based mud filtrates (OBMF).

3.2.1 T2 distributions

T2 distributions by the ILT1 method and Anahess/ILT method are plotted in Figure 2. The effect of varying regularization factors for ILT1 and broadening factors of Anahess/ILT is shown. As seen from ILT1 distributions, only when the regularization factor is considerably small do the two peaks start to be separated. These peaks, however, are well separated over the large range of broadening factors used for the Anahess/ILT method. Thus, the Anahess/ILT method quantifies the amounts of different fluids directly without any curve fitting and guessing in most cases and generates continuous distributions. In case peaks overlap with the Anahess/ILT method, the discrete components of the peak can still be identified by the Anahess method. The T2 of the brine is 1.995 seconds By ILT1 (R=0.001) and 1.861 seconds by the Anahess method, while the peak T2 value of 10 ml of the same brine (not shown) is between 1.778 and 1.995 By ILT1 (R=1), indicating that simply adjusting the ILT regularization factor does not guarantee accurate single relaxation time if needed. Anahess method returns two discrete components corresponding to two major peaks by ILT1 and a much smaller component with T2 of 0.134 seconds, which are labeled with dashed lines of the Anahess/ILT graph in Fig. 2. When varying the broadening factor, the OBMF indicates that it is not as homogenous as the single peak by the ILT method. The OBMF appears to be composed of both light and heavy components from the distribution at broadening-3 and broadening-4, revealing more details about chemical composition. Even though the ILT method is known to be the data processing technique suitable for data with continuous distributions, it could lose the details due to the poor spectral resolution.

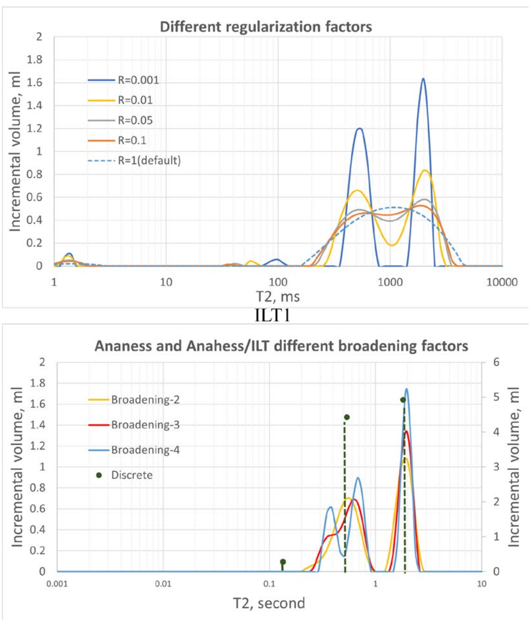


Fig. 2. The effect of varying regularization factors of ILT1 and broadening factors of Anahess/ILT.

3.2.2 2D T1-T2 distributions

The 2D T1-T2 distributions of the fluid mixture, brine, and OBMF generated by ILT1, Anahess, and Anahess/ILT method are given in Figure 3. Similar to 1D T2 distribution, the ILT method cannot differentiate the two fluids from the 2D T1-T2 data. The T2 value of brine generated by the Anahess method is 1.97 seconds, slightly larger than the one from T2. Three main components, marked with 1,2, and 3, are obtained by Anahess from the 2D T1-T2 measurement, which is the same as the 1D T2 measurement. The total volume percentage of the other peaks, marked with 4,5,6,7,8, is only 3.11%, which is negligible. Peak 4, with its T1 much less than 0.0001 seconds, and 7, with its T2 much larger than 10 seconds, are out of the plot ranges. These extremely small peaks, peaks 4, 5, 6, 7, and 8, are generated due to lower SNR and can also be ignored. The Anahess/ILT method produced a T1-T2 map with a clear separation between different fluid types and accurate volume without any adjustment, unlike data by the ILT methods.

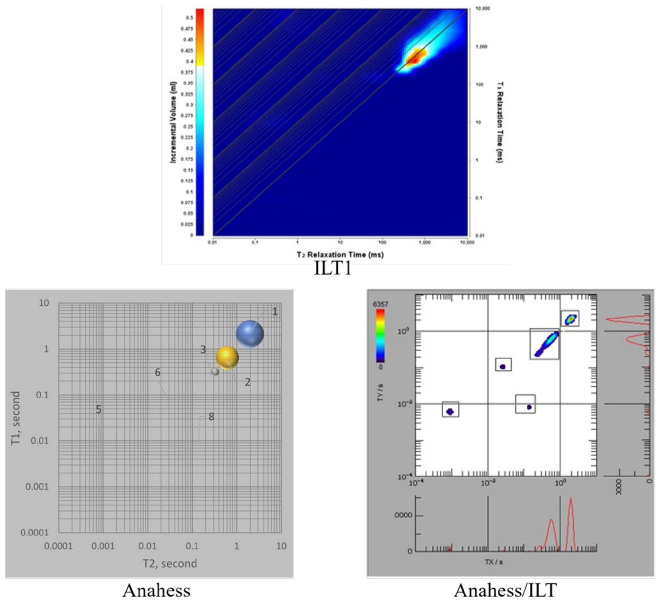
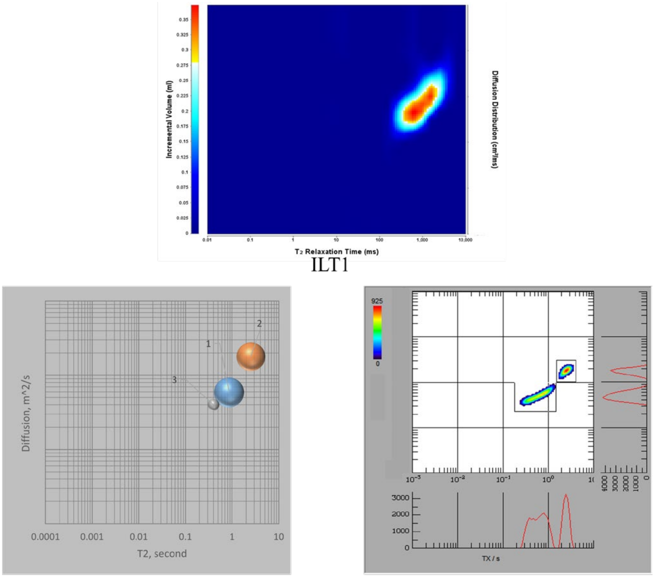


Fig. 3. 2D T1-T2 distributions of the fluid mixture.

3.2.3 2D T2-D distribution

2D T2-D measurement is another common NMR measurement with many qualitative and quantitative applications. The 2D T2-D distributions processed by ILT1, Anahess, and Anhess/ILT are given in Figure 4. The fluids cannot be differentiated from the ILT map; the same three components are obtained by the Anahess method, and the map by Anahess/ILT clearly shows how the T1 and diffusion coefficients of filtrate vary, which may provide more accurate T2-D-based quantitative analysis such as surface relaxivity (23).



ILT1

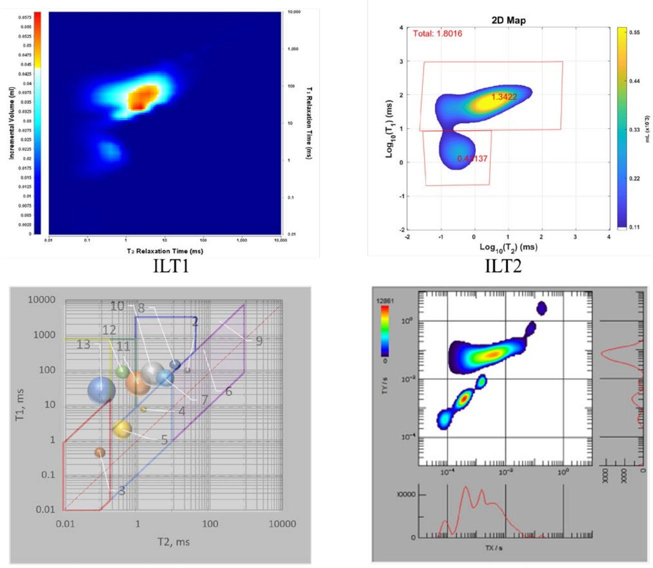
Anahess

Anahess/ILT

Fig. 4. T2-D distributions of the fluid mixture.

3.3 Shale sample

The new NMR shale Fluid Discretization Method (NFDM) workflow has, for the first time, been applied to shale samples, with the results compared and verified with both other NMR and conventional methods. The strength of DI-based NFDM is evident for the samples with severely overlapping NMR data on 2D T1-T2 maps. The results of the 2D T1-T2 data processed by ILT and Anahess methods for the shale sample are shown in Figure 5.



ILT1

ILT2

Anahess with fluid type scheme

Anahess/ILT

Fig. 5. T1-T2 distributions of the shale sample.

3.3.1 2D T1-T2 distributions

The 2D T1-T2 distributions (ILT1, ILT2, Anahess with fluid type scheme, and Anahess/ILT) of the shale sample are presented in Figure 5. The 3D bubble graph (Anahess with fluid type scheme of Figure 5) has a general 2D T1-T2 fluid typing scheme added for demonstration of NFDM workflow, which should be tuned to the specific unconventional reservoir. Unlike fluid typing based on the 2D map by the ILT methods with user-determined manual cut-off values, curve fitting, or machine learning methods, the NFDM workflow simply assigns discrete components to fluid types based on their relaxation times for the specific formation. The result of discrete fluid type assignment and the volumes by NFDM is shown in Table 3. The existing methods of manual cut-off and machine learning may still work on this example, however, with low efficiency, large uncertainty, and low spectral resolution. With discrete component signatures by the DI-NMR method, the assigning and grouping of components is direct and robust. On the contrary, applying the regular or irregular boundaries by either manual cut-off or machine learning methods to the data with continuous distribution of various fluid types does not guarantee consistent data interpretation.

Table 3. Fluid volumes of the shale sample.

Fluid type	Oil-Bitumen/ Heavy oil	Oil-Absorbed	Oil-free	water-structural and absorbed	water-free	Other-noise
Discrete component number	13	12	7,8, 10,1 1	3	2,4,5,6	1,9
Volume (ml)	0.273	0.138	0.77 7	0.107	0.245	0.073

4 Conclusion

The review of the various NMR data inversion methods reveals that they inherently impose constraints on the results, making it essential to apply them in suitable application cases. For the purpose of fluid typing and saturation determination, the proposed NMR data processing method, DI-NMR, provides a new potential workflow that is robust and accurate. We successfully demonstrated the application of the proposed shale fluid typing method (NFDM), DI-NMR workflow based on the Anahess method, for accurate fluid typing and saturation determination substantiated by the preliminary results of different samples. Besides fluid typing from 2D T1-T2 data, new applications may be developed by combining the continuous distributions from the ILT methods and discrete components from DI methods. More applications in reservoir assessment and well producibility evaluation using the proposed method will be continuously tested. Other quantitative applications of using the discrete inversion method alone and the inversion methods combining both discrete and continuous features are also under investigation. Finally, the developed technologies, DI-NMR for data processing and NFDM for fluid typing and quantifications, are currently being tested with logging data for both conventional and unconventional reservoirs.

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