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EVALUATION OF THE INFLUENCE OF SIGNAL-TO-NOISE RATIO IN OIL ANALYSIS BY TD-NMR: COMPARISON BETWEEN ILT AND KBDM

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Abstract: Time-Domain Nuclear Magnetic Resonance (TD-NMR) has been gaining prominence in industry, delivering faster, more accurate, and relatively cheaper results compared to classical analytical methods. TD-NMR technique is based on the determination of longitudinal (T_1) and transverse (T_2) relaxation times. The T_2 relaxation time is more commonly used because it can be obtained in a single shot using the CPMG pulse sequence. This study aimed to process CPMG decay data using two methods: Inverse Laplace Transform (ILT) and Krylov Basis Diagonalization Method (KBDM). The data were collected from three different oil samples using two different instruments: the SpecFIT HR 50 and the Minispec. The results show that ILT and KBDM provide similar T_2 values, indicating that both techniques are consistent. However, KBDM proved to be much more susceptible to equipment noise than ILT, which becomes evident when using an instrument with a lower signal-to-noise ratio.

Keywords: TD-NMR, ILT , KBDM, signal processing.

ANÁLISE DA INFLUÊNCIA DE RELAÇÃO SINAL-RUÍDO NA ANÁLISE DE ÓLEO POR RMN-DT: COMPARAÇÃO ENTRE ILT E KBDM

Resumo: A Ressonância Magnética Nuclear no Domínio do Tempo (RMN-DT) vem ganhando destaque na indústria, oferecendo resultados mais rápidos, precisos e relativamente mais baratos em comparação com os métodos analíticos clássicos. A técnica de RMN-DT baseia-se na determinação dos tempos de relaxação longitudinal (T_1) e transversal (T_2). O tempo de relaxação T_2 é mais comumente utilizado, pois pode ser obtido em uma única aquisição utilizando a sequência de pulsos CPMG. Este estudo teve como objetivo processar os sinais de decaimento CPMG utilizando dois métodos: a Transformada Inversa de Laplace (ILT) e o Método de Diagonalização por Base de Krylov (KBDM). Os dados foram coletados a partir de três diferentes amostras de óleo, utilizando dois instrumentos distintos: o SpecFIT HR 50 e o Minispec. Os resultados mostram que ILT e KBDM fornecem valores de T_2 semelhantes, indicando que ambas as técnicas são consistentes. No entanto, o KBDM mostrou-se muito mais suscetível ao ruído do equipamento do que o ILT, o que se torna evidente ao utilizar um instrumento com menor relação sinal-ruído.

Palavras-chave: RMN-DT, ILT, KBDM, processamento de sinais.

1. Introduction

TD-NMR is a widely used technique, as it is a non-destructive analytical method capable of providing insights into the structure and molecular mobility of the sample. In industry, this technique stands out for being non-invasive and allowing rapid acquisition of results when compared to classical analytical techniques, emerging as an alternative to these methods. Analyses are carried out through longitudinal (T_1) and transverse (T_2) relaxation times. TD-NMR has been widely applied in the oil and fat industries.

Vegetable oils are composed of triacylglycerols (TAGs), formed by the esterification of three fatty acid molecules and one glycerol molecule. T_1 and T_2 relaxation times can be used to evaluate the structure and mobility of TAGs and, in this way, to verify how they behave in the sample. The distribution of T_1 and T_2 values can be obtained through mathematical processing using NMR signals. There are several types of processing methods, but those evaluated in this study are the Inverse Laplace Transform (ILT) and the Krylov Basis Diagonalization Method (KBDM).

2. Materials and Methods

Initially, three types of oils — canola, corn, and soybean — obtained from commercial sources were selected and analyzed using the Minispec (Bruker, Germany) and SpecFit HR 50 (Fine Instrument Technology, São Carlos-SP) instruments to obtain CPMG signals. The data obtained from the CPMG signals were processed after performing an averaging grouping, aiming to reduce the number of variables. The reduced signal was used to apply the KBDM method in Origin 8.5 software, using the script proposed by Moraes et al. (2014). The same signals were also analyzed using the ILT processing method developed in Python, which incorporates Tikhonov regularization and was implemented within the Origin 8.5 software, as described in Moraes (2021).

3. Results and Discussion

The CPMG signals obtained from the three oil samples were processed using ILT and KBDM, from which the distribution graphs of transverse relaxation times were generated, as shown in Figure 1. Figure 1 a) presents the results obtained with the SpecFit HR 50, while Figure 1 b) corresponds to the results obtained with the Minispec. Figures 1 a) and 1 b) show the graphs generated using the ILT method, in which a tri-exponential behavior is observed, in agreement with what was reported by Robinson & Cistola (2014), who identified such behavior in mono- and polyunsaturated fatty acids. The graphs in Figures 1 a) and 1 b) also show the T_2 relaxation time distribution obtained using the KBDM method, also revealing a tri-exponential behavior, which corroborates the results obtained with ILT.

As can be observed, Figure 1 a) shows a greater agreement in the T_2 distribution between the methods used when compared to the results in Figure 1 b), obtained with the Minispec. The difference between these results occurs because the KBDM method is an ill-posed problem and is highly sensitive to the signal-to-noise ratio.

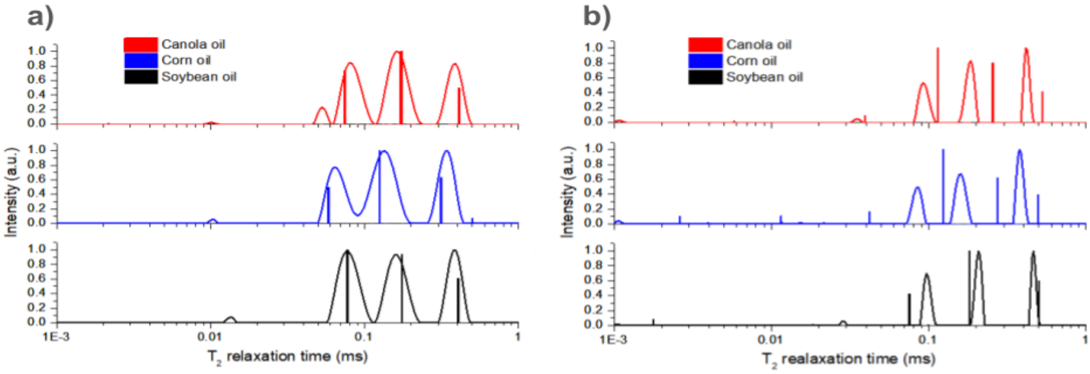

Figure 1: Difference between the three types of oils with different CPMG signal processing methods using different instruments. a) Using ILT and KBDM methods with the SpecFit HR 50 instrument; b) Using ILT and KBDM methods with the Minispec instrument.

Therefore, this ratio was calculated as the ratio between the first and the last point of the CPMG signals for each sample using both instruments. These values are presented in Table 1.

Table 1: Signal-to-noise ratio for the different samples analyzed with the SpecFit HR 50 and the Minispec.

	Signal-to-noise ratio	
Sample	SpecFit HR 50	Minispec
Canola oil	2612	202
Corn oil	2865	461
Soybean oil	2879	140

4. Conclusions

The ILT and KBDM methods used in this work showed good results for the experimental signals of the analyzed oil samples. There was good agreement between the results, as both methods presented very similar distributions of T_2 values, which allows us to affirm that these two methods are complementary. However, the KBDM method exhibited quite discrepant T_2 values when applied to instruments with a low signal-to-noise ratio.

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