12th NUCLEAR MAGNETIC RESONANCE USERS MEETING

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EXTENDED ABSTRACTS BOOK

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ANALYSIS OF RELAXATION TIMES IN FLOW CWFP-NMR

Antonio Marchi Netto[1, 2*], Luiz Alberto Colnago[2]
[1] *Instituto de Física de São Carlos, University of São Paulo*
[2] *EMBRAPA Instrumentação Agropecuária*
**netto@cnpdia.embrapa.br*

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Recently, it was demonstrated that online NMR using continuous wave free precession (CWFP) pulse sequence is a fast and powerful tool for quantitative measurements (1). The method has been applied for analysis of oilseeds with similar relaxation times. For the analysis of oilseed with different chemical composition, the influence of the relaxation time in the CWFP signal amplitude has been studied. In this paper, we evaluate, experimentally and theoretically, the influence of the relaxation times in the quantitative measurement by online CWFP. The intensity of CWFP signal in flowing samples depends on the flip angle (α), offset angle (ψ), relaxations times (T_1 and T_2), magnetic field gradient (G), sample velocity (v) and pulse repetition time (T_p).

The steady-state (SSFP) simulation through the Monte Carlo method (2) fails for large values of T_2/T_p that is a crucial point for obtaining the CWFP condition. Hence, we had employed a different approach detailed in a previous work (3). The CWFP sensitivity to flow can be described by direct iterations of Bloch matrices.

In this theoretical description the radio frequency pulses on the x-axis are considered simple instant rotations on this same axis. The magnetic field B_0 is taken as a normalized Lorentz distribution, however initial simulations indicate that in the CWFP sequence inhomogeneity fields does not influence the signal, once having reached the state. In this case, the use of very small angles $\Delta\psi=\Delta\omega T_p=T_p/T_2^*$ becomes necessary, which are obtained with $T_p=0.3msec$ and $T_2^*=20msec$, already indicating that it will not be necessary an integration of the offsets.

Bloch's equations for static samples magnetization in the steady state were first outlined by Freeman and Hill (4), but now it shows the needed an addition of a term $\phi=\gamma G v T_p^2$ for each new cycle of iteration between each echo times (3), represented by the following equation:

$$\vec{M}_{n+1} = \hat{R}(n,\phi,\psi)\vec{M}_n + (1-E_1)M_0 \tag{1}$$

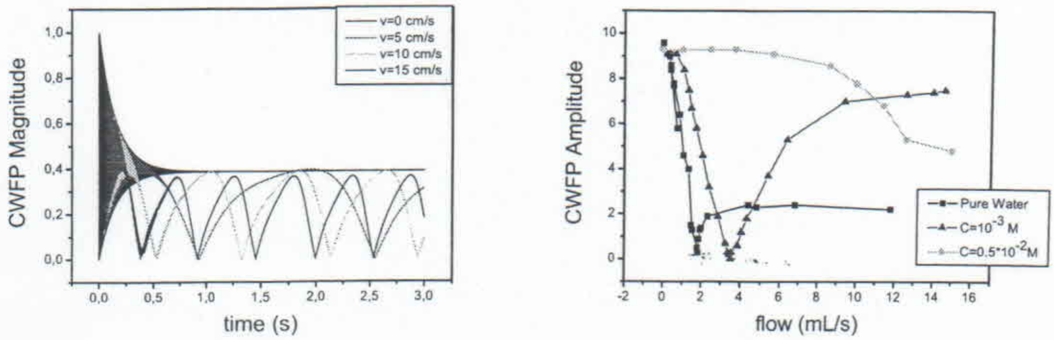
where $R(n,\phi,\psi)$ addresses both the rotation due the *rf*, the precession angle and the relaxations times, given by:

$$\hat{R}(n,\phi,\psi)=\begin{bmatrix}\cos(\psi+n\phi) & \sin(\psi+n\phi) & 0\\ -\sin(\psi+n\phi) & \cos(\psi+n\phi) & 0\\ 0 & 0 & 1\end{bmatrix}\times\begin{bmatrix}E_2 & 0 & 0\\ 0 & E_2 & 0\\ 0 & 0 & E_1\end{bmatrix}\times\begin{bmatrix}1 & 0 & 0\\ 0 & \cos\alpha & \sin\alpha\\ 0 & -\sin\alpha & \cos\alpha\end{bmatrix} \tag{2}$$

Numerical simulations show, in general, a real state of the magnetization in the *xy* plan is achieved for *n* greater than $5T_1/T_p$, as a n periodic function with oscillation period $\Delta n=2\pi/\phi$, with phase governed by ψ and amplitude controlled by ϕ (figure 1a).

Under these conditions, a wavelength on the conditions of the problem $\lambda=2\pi/\gamma G T_p$ is much greater when compared to the coil size l is obtained, so a very uniform magnetization space is expected. A better analysis shows all magnetization components of the sample between n as soon the sample gets in, as soon the sample gets out are equivalent, so the dominant contribution is given by the term M_n with n in the range of $2\pi m/\phi$, with m big enough to satisfy the condition $2\pi m/\phi>5T_1/T_p$ necessary to achieve the steady-state.

The simulation and experimental results obtained with water plus relaxing agent in several concentrations show a strong dependence on the amplitude of CWFP signal and the relaxation times, as shown in the figure 1b.



(a) (b)

Figure 1: a) Simulated CWFP signals for vegetal oil (T_1=199.6ms, T_2= 127ms), at a field gradient = 97mG/cm and T_p= 300μs; b) Experimental results for water plus relaxing agent.

This detailed study on the flow regime in CWFP was important for the optimization of quantitative determination of oil content in seeds by online NMR.

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