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Constrained Optimized Water Suppression (COWS) for ¹H Magnetic Resonance Spectroscopy

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Synopsis

Water suppression is a necessary component to magnetic resonance spectroscopy experiments due to its roughly 5000-fold higher intensity than the metabolites of interest. Here we introduce a novel algorithm for water suppression which operates in a similar manner to that originally proposed by WET and expanded upon by VAPOR, but is flexible in that it can accommodate an arbitrary number of RF pulses, minimum duration between pulses, total module duration and maximum flip angles. This method is referred to as Constrained Optimized Water Suppression. We demonstrated the improvement of COWS over the gold standard VAPOR in simulations and in vivo.

Introduction

The concentration of water is ~5000x larger than the concentration of metabolites in in vivo MRS, thus to visualize and quantify the metabolites water suppression (WS) modules substantially reduce the measured water signal. The gold standard for water suppression is Variable Power Radio Frequency Pulses with Optimized Relaxation Delays¹ (VAPOR). Although outstanding WS was attained in the original VAPOR manuscript¹ and certain subsequent implementations²⁻⁵, there can be found numerous examples in the literature of suboptimal WS with VAPOR⁶⁻⁸, and as such subsequent modules have been developed in an attempt to out-perform VAPOR, such as HGWS⁷. Additionally, even VAPOR schemes which have been shown to provide high-quality water suppression in metabolite scans⁵ result in poor water suppression for macromolecule spectra due to the double-inversion preparation module⁹. Constrained Optimized Water Suppression (COWS) enables the optimization of a WS scheme tailored to the details of the MRS experiment at hand with number of RF pulses, minimum duration between pulses, total module duration and maximum flip angles as input constraints. An implementation of the COWS algorithm has been made available to the scientific community free of charge (http://innovation.columbia.edu/technologies/CU21111_COWS).

Methods

COWS Algorithm

The longitudinal magnetization after a series of n RF pulses can be expressed as^{10,11}

$$M_z^n(\boldsymbol{\tau}, \boldsymbol{\theta}, T_1, F_B) = M_z^{n-1} \cos(F_B \theta_n) e^{-\tau_n/T_1} + M_z^{eq} (1 - e^{-\tau_n/T_1}), [1]$$

where T_1 is the longitudinal relaxation time, if n=0 then M_z^0 is the longitudinal magnetization prior to the pulse, M_z^{eq} is the equilibrium longitudinal magnetization and F_B is the B₁ overdrive factor (i.e., the factor by which the flip angle deviates from its nominally prescribed value due to B₁ inhomogeneities), $\boldsymbol{\theta}$ and $\boldsymbol{\tau}$ are the vectors of the flip angles and delays after the pulse. The initial value for the longitudinal magnetization prior to the WS module, $M_z^{0,initial}$ is assumed to be equal to M_z^{eq} . The cost function for COWS is

$$C(\boldsymbol{\tau}, \boldsymbol{\theta}) = \sum_{i=1}^{N_{T_1}} \sum_{j=1}^{N_{F_B}} M_z^n(\boldsymbol{\tau}, \boldsymbol{\theta}, T_{1,i}, F_{B,j}) \exp \left(- \left(\frac{T_{1,i} - \bar{T}_1}{W_{T_1}} \right) - \left(\frac{F_{B,j} - \bar{F}_B}{W_{F_B}} \right) \right), [2]$$

where M_z^n is calculated via Equation 1, $T_{1,i}$ is the ith T_1 value, and $F_{B,j}$ is the jth B₁ overdrive factor. The exponential is a Gaussian weighting function to provide greater weight to the values closer to the mean values and the overbar is used to denote the mean. The optimized flip angles and delays were then calculated via

$$[\boldsymbol{\tau}^{COWS}, \boldsymbol{\theta}^{COWS}] = \text{argmin}_{\boldsymbol{\tau}, \boldsymbol{\theta}} (C(\boldsymbol{\tau}, \boldsymbol{\theta})). [3]$$

The numerical optimization was performed using the active set method with constraints in MATLAB (Mathworks, Natick, MA) R2013b.

COWS Modules

Two COWS WS modules were developed and tested here. The first utilized 7 pulses, similar to VAPOR¹, but with substantially reduced module duration (236 ms), referred to as COWS(7;236). The second employed an equal module duration to VAPOR (626 ms), but utilized 12 pulses, referred to as COWS(12;626). The default values $\bar{W}_{T_1} = 3s$ and $\bar{W}_{F_B} = 0.1$ were used and the range of values considered were $0.5s \leq T_1 \leq 5.0s$ and $0.75 \leq F_B \leq 1.25$. The minimum duration of 28 ms between successive WS pulses, and 21 ms duration between the final water suppression pulse and the excitation pulse were used due to experimental constraints. The crusher scheme to dephase all water coherence pathways is automatically obtained from COWS via DOTCOPS^{12,13}. The pulse sequence for COWS(7;236) and conceptual diagram of action is given in Figure 1.

The water suppression efficiency was calculated as

$$f_{ws} = \frac{\max(|S_{sup}|)}{\max(|S_{unsup}|)}, [4]$$

where $|S_{sup}|$ is the absolute (i.e., magnitude) spectrum with the water suppression module on in the spectral range of water (4.60 to 4.70 ppm) and $|S_{unsup}|$ is absolute spectrum of the water reference.

Experimental Validation

One healthy subject was scanned with informed consent with TE/TR = 20 ms/2000 ms sLASER^{5,14,15} acquisition at Siemens Prisma 3 T (Siemens Healthineers, Erlangen, Germany) with 32-channel head coil. Metabolite spectra in the occipital and prefrontal lobe were collected using three WS schemes: VAPOR, COWS(7;236) and COWS(12;626). Macromolecule spectra obtained with a double inversion preparation module, T1 = 920 ms, T2 = 330 ms in the parietal lobe were also acquired using VAPOR and COWS(7;236).

Results and Discussion

The flip angles (FA), delays for both COWS schemes and the VAPOR implementation are given in Table 1. Bloch simulations demonstrate COWS(7;236) and COWS(12;626) demonstrate substantially improved water suppression over the range of simulated T_1 and B_1 values (Figure 2). The specific absorption rate (SAR) compared to VAPOR

was 0.66 and 1.36 for COWS(7;236) and COWS(12;626), respectively. Substantially improved water suppression was obtained for both the metabolite and macromolecule voxels (Figure 3). The water suppression efficiency was 0.22%/0.22%/0.08% for VAPOR, COWS(7;236) and COWS(12;626), respectively, for the occipital lobe, and, 0.29%/0.15%/0.06% for the parietal lobe. VAPOR and COWS(7;236) had comparable performance despite the substantially reduced module duration and reduced SAR, and substantial improvement of COWS(12;626) over VAPOR which have equal module duration. The macromolecule spectra acquired with double inversion recovery nulling of metabolites from COWS had considerably reduced residual water (Figure 4), with a water suppression efficiency of 2.43% for VAPOR and 0.57% for COWS(7;236).

Conclusions

A WS algorithm was developed and tested versus the current state-of-the-art WS scheme, VAPOR. Improved water suppression was demonstrated for both schemes, with COWS(12;626) providing the WS of choice for metabolite spectra. COWS(7;236) provided improved water suppression over VAPOR for macromolecule spectra, with a substantially reduced module duration.

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Figures

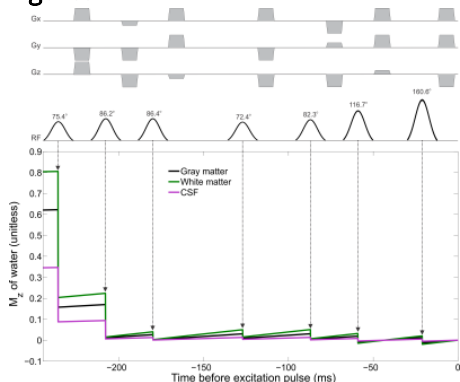


Figure 1: Pulse sequence and mechanism of action for COWS(7;236) with TR = 2 s. A Bloch simulation demonstrating that even for tissues with drastically different T_1 relaxation times¹⁶ the longitudinal magnetization is effectively suppressed at the time of excitation. COWS does not assume equilibrium magnetization (i.e., complete relaxation between successive TRs), as can be seen by how the three different tissue-types have a different steady-state magnetization.

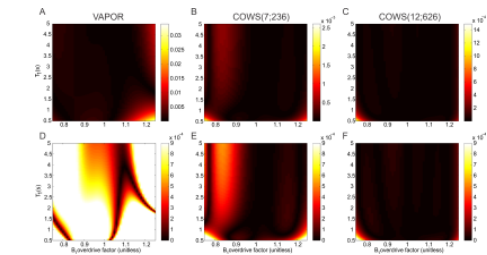


Figure 2: Bloch simulations of the residual longitudinal water magnetization (unitless) after the water suppression schemes for VAPOR, A/D, COWS(7;236) B/E, and COWS(12;626), C/F. Note the differences in image scale in the top row. The data in the second row is identical to the data in the first row, with a constant window/level across all three different water schemes to demonstrate the marked improvement in COWS over VAPOR.

	Pulse Number	1	2	3	4	5	6	7	8	9	10	11	12
COWS(7;236)	Delay	28,000	28,000	53,052	99,764	28,000	98,234	21,000					
	FA [°]	75.4	86.2	86.4	72.4	82.3	136.7	100.6					
	Delay	150,000	80,000	160,000	80,000	100,000	30,000	26,000					
VAPOR	Delay	90.0	90.0	160.2	90.0	160.2	90.0	160.2	62,789	87,689	28,000	44,538	21,553
	FA [°]	75.8	3.4	110.6	141.1	180.0	20.1	89.6	76.3	117.2	79.6	127.7	167.6
	Delay	82,664	28,000	30,553	28,000	61,301	51,238	99,234	62,789	87,689	28,000	44,538	21,553
COWS(12;626)	Delay	82,664	28,000	30,553	28,000	61,301	51,238	99,234	62,789	87,689	28,000	44,538	21,553
	FA [°]	75.8	3.4	110.6	141.1	180.0	20.1	89.6	76.3	117.2	79.6	127.7	167.6
	Delay	82,664	28,000	30,553	28,000	61,301	51,238	99,234	62,789	87,689	28,000	44,538	21,553

Table 1: Flip angles (FA) and delays for the two COWS schemes developed and tested here as well as the VAPOR¹ scheme used for comparison.

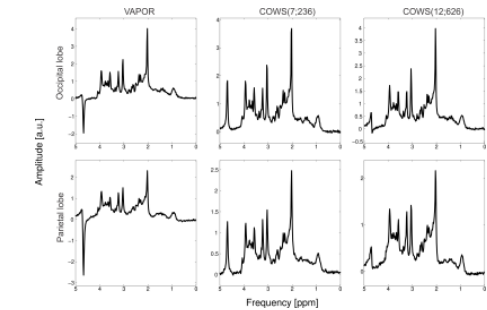


Figure 3: Metabolite spectra obtained from the occipital lobe (top row) and parietal lobe (bottom row) for the three water suppression schemes tested here, VAPOR, COWS(7;236) and COWS(12;626). COWS(7;236) has comparable performance to VAPOR, while COWS(12;626) has marked improvement over both. Note that WS schemes were applied as theoretically optimized and no experimental fine tuning was performed.

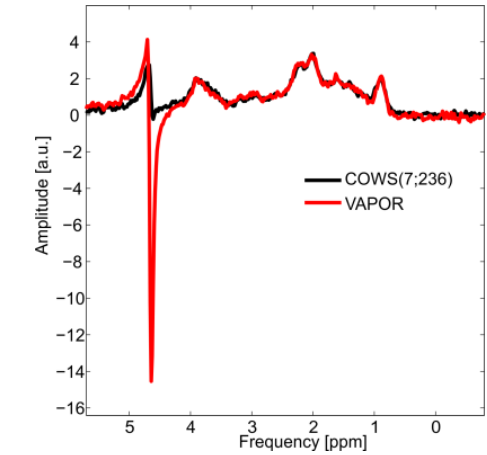


Figure 4: Macromolecule spectra obtained from the parietal lobe for VAPOR (red) and COWS(7;236) (black). Marked reduction of residual water for COWS(7;236) was observed over VAPOR. COWS(12;626) was not used due to its interference with the double inversion preparation module.