CESTsimu: A User-Friendly GUI for spectral and spatial CEST simulation

Huabin Zhang[1,2], Bensheng Qiu[1], Jianpan Huang[2*]

*[1] Medical Imaging Center, Department of Electronic Engineering and Information Science, University of Science and Technology of China, Hefei, China; [2] Department of Diagnostic Radiology, The University of Hong Kong, Hong Kong, China; * Corresponding Author.*

INTRODUCTION: Simulation based on the Bloch-McConnell Equation (BME) plays a pivotal role in the advancement of Chemical Exchange Saturation Transfer (CEST) MRI technology by providing a digital tool for optimizing sequence protocols and post-processing techniques.[1-5] Various CEST simulation software packages, such as MRiLab[6], Pulseq-CEST[7], and CALF[8] have been developed for CEST simulation or post- processing. However, these tools either involve complex sequence definition procedures or lack a user-friendly graphical user interface (GUI), which hinders the implementation of CEST simulation by users without extensive knowledge of CEST physics. Recently, the Bloch-McConnell simulation (BMsim) challenge has been established, with the goal of standardizing CEST simulation[9]. However, results from different research groups exhibited variation. In this study, we have developed a user-friendly GUI called CESTsimu that enables intuitive spectral (1D Z-spectrum) and spatial (2D phantom) CEST simulations. We anticipate that CESTsimu will enhance the accessibility and reliability of CEST simulations, thus promoting the broad utilization of CEST MRI among diverse users.

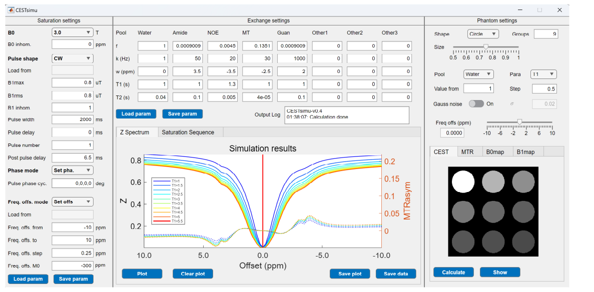

Fig. 1. GUI interface of CESTsimu App, consisting of three panels: 'Saturation settings', 'Exchange settings', and 'Phantom settings'.

METHODS: CESTsimu has been developed on MATLAB App Designer and employs analytical calculations to simulate the evolution of the magnetization vector from the BME using matrix exponential techniques.[10] The GUI allows users to easily manipulate CEST parameters within both the 'Saturation settings', 'Exchange settings', and 'Phantom settings' modules (Fig. 1). Additionally, users have the option to expedite the configuration of simulation experiment parameters by importing pre-stored files from CESTsimu or Pulseq-CEST. CESTsimu provides both spectral (1D Z-spectrum) and spatial (2D phantom) CEST simulations. Within the 2D phantom module, users can customize Gaussian noise distribution, phantom dimensions, and quantitative parameters pertaining to contrast experiments through the GUI interface. Simulation outcomes are presented directly within the GUI, while users retain the capability to export and save the experimental parameters and simulation results. To demonstrate the functions of CESTsimu, two experiments were conducted using a five-pool model[11] that included magnetization transfer (MT), amide, nuclear Overhauser enhancement (NOE), and guanidino. In experiment 1, we varied the saturation settings (B_0, B_1 and T_{sat}) while keeping the exchange settings constant (amide k and f). In experiment 2, we varied the exchange settings while keeping the saturation settings constant.

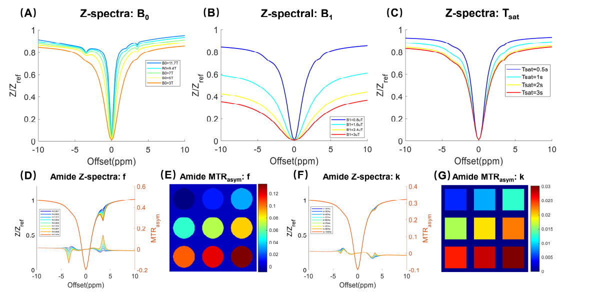

Fig. 2. Simulation of various saturation settings (A-C), amide fraction f (D-E), and amide exchange rate k (F-G).

RESULTS & DISCUSSION: In experiment 1, Figs. 2A illustrates that as B_0 increases, the CEST peaks exhibit increased sharpness, demonstrating improved spectral resolution. Figs. 2B demonstrates that an increase in B_1 amplifies the degree of MT saturation which dilutes other CEST effects. Figs. 2C primarily elucidates that a higher saturation time (T_{sat}) leads to increased CEST/MT saturation until reaching a steady-state. These results from the varied scanner settings elucidate the capability of CESTsimu in optimizing sequence parameters. In experiment 2, the increases of amide f from 0.001 to 0.009 result in the increases of +3.5 ppm MTR_{asym} signal from -0.009 to 0.136 (Figs. 2D-E). The increases of amide k from 20 Hz to 100 Hz also correlates with elevations in the MTR_{asym} values from -0.022 to 0.003 (Figs. 2F-G). These findings illustrate the ability of CESTsimu to accurately mimic CEST experiments under diverse exchange pool and environmental conditions.

CONCLUSION: We developed a user-friendly GUI for intuitive CEST simulation. Users can easily perform CEST simulation experiments with varied saturation and exchange settings. Experimental results demonstrate that CESTsimu is capable of mimicking CEST experiments under diverse exchange pool and environmental conditions, thereby facilitating the broad utilization of CEST MRI among diverse users.

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