POM: A Simulation Program for NMR under Inter- and Intramolecular Interactions

C. Cai[1], Z. Chen[1,2], S. Cai[1], J. Zhong[2]

[1]Departments of Physics and Communication Engineering, Xiamen University, Xiamen, Fujian, China, People's Republic of, [2]Departments of Radiology and Biomedical Engineering, University of Rochester, Rochester, NY, United States

Introduction

Computer simulations are often essential to the development and understanding of the physical nature of NMR experiments [1]. Quite a few simulation software packages have been developed, such as BlochLib [1] and Qsim [2]. However, a convenient and efficient method is still lacking for the simultaneous simulation of macroscopic effects such as dipolar field and radiation damping, and microscopic effects such as scalar couplings. To solve this problem, we introduced the product operator matrix (POM) method, which enables us to deal with scalar couplings in the frame of the non-linear Bloch equations [3]. The POM program established accordingly was programmed using Visual C++ with a graphical user interface. The program is easy to use, fast, and can simulate variety of effects in liquid state spin-1/2 NMR 1D or 2D experiments.

Functions

The POM program can be used for one- and two-dimensional (1D and 2D) spectral simulation of spin-1/2 systems in liquid NMR with or without scalar couplings (the sample can be 1D or 3D), and for simulations of related magnetic resonance imaging (MRI) experiments. A graphical interface is included for input and output, data treatment, and analysis. Effects of diffusion, relaxation, scalar couplings, dipolar field, chemical shifts, inhomogeneous field, radiation damping, and RF pulses can be taken into account together. Simulation algorithms can be simplified when some approximations are assumed. For example, in the simulation of normal liquid, the calculation can be simplified to 1D case if the gradient field is only along the z axis. If radiation damping can be further ignored, the fifth-order Cash-Karp Runge-Kutta formulism can be simplified in resolving the nonlinear Bloch equations. Simplified algorithms are especially helpful for 2D spectral simulation which takes much CPU time. It takes about 5 hours to get a 2D simulation spectrum of an I_2S_3 spin system (512 points in indirect dimension and 1024 points in direct dimension, 1D sample (AMD CPU 2500+, 512M memories). The program provides some basic display functions: 1D and 2D spectra, the pulse sequence diagram, images from MRI, and the display of array spectra.

Operations

All of the simulation can be operated within the graphical user interface shown in Fig.1. Complex RF pulse sequences can be simulated using "Add Seq" or "Sub Seq" button. The RF pulses can be selective, non-selective, or saturation RF pulses. The information of the spin system can be set by "Spin System" button. "IS", "IS_2", "IS_3", "I_2S_2", and "I_2S_3" spin systems are now available, and more different types of spin systems can be included easily. The spin system can also be hetero-nuclear, such as C-H coupling system. The information of pulse sequence and spin system can be saved and retrieved. By pressing the "New Task" button, different simulation tasks can be pended to a series of tasks waiting for simulations. For batch tasks, such as DOSY spectral simulation, the "Array Simul" button can be used.

Example

The RF pulse sequence shown in Fig.2 was applied on a $CHCl_2CH_2Cl$ sample. This sequence can produce signals from both inter-molecular dipolar couplings and intra-molecular scalar couplings synchronously, thus makes the resulted 2D spectra rather complicated, as seen in Fig.3. The multiplicity patterns of the cross-peaks are complex and different from the multiplicity patterns of normal inter-molecular or intra-molecular multiple quantum coherence peaks. Simulation results are coincident with the experimental ones.

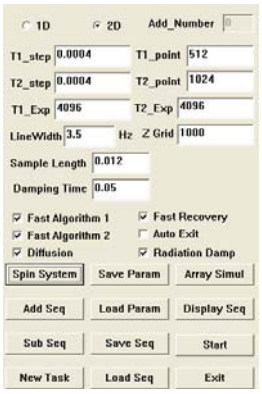

Fig.1 The main control panel of the POM program.

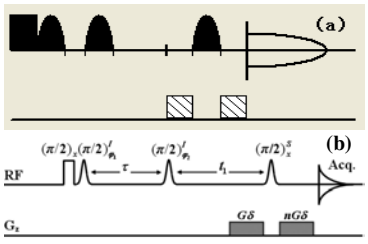

Fig.2 An example of pulse sequence: (a) the sketch provided by the POM program; (b) the corresponding pulse sequence.

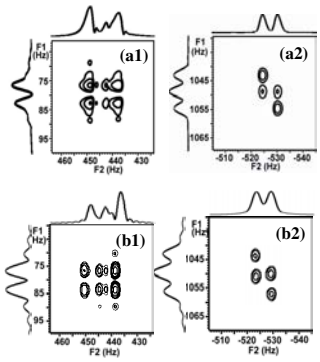

Fig.3 The expanded regions of cross-peaks in 2D double-quantum coherence spectra of $CHCl_2CH_2Cl$: (a) experimental spectra; (b) simulation spectra.

Conclusion

In this work, a new convenient and efficient NMR simulation tool, POM, was introduced. It is helpful for designing new pulse sequences and analyzing the experimental results, especially when distant dipolar field, radiation damping field, and scalar couplings are all needed to consider. In such case, the inter-molecular multiple quantum coherences and intra-molecular multiple quantum coherences coexist [4], which makes the spectra very complex and difficult to analyze by theoretical methods alone.

Acknowledgment

This work was partially supported by the NNSF of China under Grants 10234070 and 20573084, and NIH under Grant NS41048.

References

[1] Blanton WB. J. Magn. Reson. 162 (2003) 269-283.
[2] Helgstrand M, et al. J. Biomolecular NMR 30 (2004) 71-80.
[3] Cai CB, et al. J. Magn. Reson. 172 (2005) 242-253.
[4] Zhu XQ, et al. Physica B 362 (2005) 286-294.