

# Theoretical Model for XTC (Xenon Transfer Contrast) Experiments with Hyperpolarized $^{129}\text{Xe}$

M. I. Hrovat<sup>1</sup>, I. Muradian<sup>2</sup>, E. Frederick<sup>3</sup>, J. P. Butler<sup>4</sup>, H. Hatabu<sup>2</sup>, and S. Patz<sup>2</sup>

<sup>1</sup>Mirtech, Inc., Brockton, MA, United States, <sup>2</sup>Radiology, Brigham and Women's Hospital, Boston, MA, United States, <sup>3</sup>Dept. of Physics, University of Massachusetts at Lowell, Lowell, MA, United States, <sup>4</sup>Harvard School of Public Health, Boston, MA, United States

## Introduction

XTC (Xenon polarization Transfer Contrast) is a technique which probes the exchange of gaseous  $^{129}\text{Xe}$  in the lung with dissolved  $^{129}\text{Xe}$  in the parenchymal tissue in the lung. The technique enhances sensitivity by transferring polarization from the large gas phase reservoir to the dissolved phase. Thus the exchange process is interrogated by the reduction in the gas phase signal.[1-3] CSSR (Chemical Shift Saturation Recovery) is a competing technique which also interrogates the exchange process but by direct observation of the dissolved phase.[3] CSSR has an advantage in that diffusion models may be directly applied to experimental results. The XTC method has greater sensitivity but lacks a sound theoretical foundation. To this end, we present a theoretical model that is applicable to the XTC method.

## Theory

The XTC experiment measures the amount of polarized  $^{129}\text{Xe}$  spins in the gas phase after a series or train of constant flip angle pulses (usually  $180^\circ$  pulses) separated by a characteristic exchange time,  $\tau$ . Let  $m(x,t)$  be the longitudinal magnetization at any position,  $x$ , or time,  $t$ , during the XTC experiment. We will show that  $m(x,t)$  may be well approximated by a series of terms of which each term is a solution to a well defined diffusion problem,  $dc(x,t)/dt = D d^2c(x,t)/dx^2$ .  $c(x,t)$  describes the longitudinal magnetization concentration for the 1D slab diffusion model subject to the following temporal conditions:  $c(x,0)=\{ 1 \text{ if } x \text{ is in gas phase, } 0 \text{ if } x \text{ is in dissolved phase } \}$ ,  $c(x,\infty)=\{ 1-\chi V_d/V_g \text{ if } x \text{ is in gas phase, } \chi \text{ if } x \text{ is in dissolved phase } \}$ , where  $V_d$  is the volume of the dissolved phase,  $V_g$  is the volume of the gas phase, and  $\chi$  is the partition coefficient. In XTC, the action of a selective rf pulse, flip angle  $\alpha$ , on the dissolved state is to produce the following longitudinal magnetization:

$$m(x, t_+) = m(x, t_-) \cos \alpha + m_g(t_-) c(x, 0) (1 - \cos \alpha) \quad [1]$$

where  $t_{\pm}$  refer to the time immediately after and before the rf pulse,  $m_g(t_-)$  represents the gas phase magnetization at time  $t_-$  which is assumed to be independent of position. This is a safe assumption as diffusion in the gas phase is sufficiently fast to level out any concentration gradients. It is important that the model for  $c(x,t)$  includes gas depletion, i.e. the gas phase is not an infinite reservoir. While the standard 1D slab diffusion model utilizes an infinite reservoir, gas depletion may be introduced in an ad hoc manner by correcting the gas phase concentration after each exchange time,  $\tau$ , or smaller unit of time. The action of the selective pulse of flip angle  $\alpha$  may be viewed as having two effects. One effect is to change all of the magnetization by the factor  $\cos \alpha$  (inversion for a  $180^\circ$  pulse) in both the dissolved and gas phase. The second effect is to introduce a new diffusive term which corresponds to a new slab diffusion problem as is demonstrated by the second term in Eq.[1]. Consequently, each rf pulse in the XTC experiment generates a new initial condition for any flip angle for which  $1-\cos \alpha \neq 0$ . Furthermore, the transverse magnetization is assumed to decay to zero before the beginning of the next rf pulse.

This process may be elucidated as in Eq[2] by considering the first few pulses in the XTC experiment.

$$\text{Initially:} \quad m(x,0) = A(x) \equiv \{ b_0 \text{ for gas phase, } \chi b_0 \text{ for dissolved phase } \} \quad [2a]$$

$$\text{Apply rf pulse (n=1):} \quad m(x,0_+) = A(x) \cos \alpha + b_0 c(x,0) (1 - \cos \alpha) \quad [2b]$$

$$\text{Allow diffusion:} \quad m(x,\tau) = A(x) \cos \alpha + b_0 c(x,\tau) (1 - \cos \alpha) \quad [2c]$$

$$\text{Apply rf pulse (n=2):} \quad m(x,\tau_+) = A(x) \cos^2 \alpha + b_0 c(x,\tau) (1 - \cos \alpha) \cos \alpha + b_1 c(x,0) (1 - \cos \alpha) \quad [2d]$$

$$\text{Allow diffusion:} \quad m(x,2\tau) = A(x) \cos^2 \alpha + b_0 c(x,2\tau) (1 - \cos \alpha) \cos \alpha + b_1 c(x,\tau) (1 - \cos \alpha) \quad [2e]$$

Each term in Eq.[2] evolves in time independently during a diffusion interval while each rf pulse adds an additional term that starts out as a new slab diffusion process. After many pulses the magnetization becomes a large sum of terms where each term involves diffusion over different exchange times. For  $180^\circ$  pulses, the terms alternately change sign which further complicates the interpretation of the XTC signal. For many pulses, the problem can now be solved by induction to give the magnetization after  $n$  diffusive exchange time periods (prior to the  $n+1$  pulse) as:

$$b_n = b_0 \cos^n \alpha + \sum_{k=0}^{n-1} b_k m_g((n-k)\tau) (1 - \cos \alpha) \cos^{n-1-k} \alpha \quad [3]$$

$$m(x, n\tau_-) = b_0 \cos^n \alpha + \sum_{k=0}^{n-1} b_k c(x, (n-k)\tau) (1 - \cos \alpha) \cos^{n-1-k} \alpha \quad [4]$$

where the  $b$ 's satisfy the recursion relation, Eq.[3], and  $b_0$  is the initial gas phase concentration. Eqs.[3,4] describe the XTC experiment for any flip angle for all times. As can be seen from Eq.[4], the XTC experiment measures contributions from a multitude of exchange times.

Alternatively, the XTC90 experiment, where  $\cos(90^\circ)=0$ , is unique in that all terms are zero except for  $k = n-1$ . Thus Eqs [3,4] simply become  $b_n = b_{n-1} m_g(\tau)$  and  $m(x, n\tau) = b_{n-1} c(x, \tau)$ . And the XTC90 experiment like the CSSR experiment reflects only one diffusive exchange time.

**Acknowledgements:** This work is supported by NIH

## References:

1. Ruppert, K; Brookeman, JR; Hagspiel, KD; Mugler, JP. MRM, 44:349-357 (2000).
2. Ruppert, K; Mata, JF; Brookeman, JR; Hagspiel, KD; Mugler, JP. MRM, 51:676-687 (2004).
3. Patz, S; Muradian, I; Hrovat, MI; Ruset, IC; Topulos, G; Covrig, SD; Frederick, E; Hatabu, H; Hersman, FW; Butler, JP. Acad. Rad., 15:713-727 (2008).