

# Modeling of super-dispersion in unsaturated porous media using NMR propagators



M. Fleury<sup>a,\*</sup>, D. Bauer<sup>a</sup>, M.C. Néel<sup>b</sup>

<sup>a</sup> IFP Energies Nouvelles, 92852 Reuil-Malmaison, France

<sup>b</sup> Université d'Avignon et des Pays de Vaucluse, UMR 1114 EMMAH, Avignon, France

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## ABSTRACT

We present a general model (SMIM) specifically designed for the interpretation of NMR velocimetry data. Extending the well-known concept of Mobile/Immobile tracer particles applied in dispersion theory, we reproduce two mechanisms responsible for non-Gaussian behavior: immobile molecules trapped in non-flowing zones, and unexpectedly long but rare displacements. From the derived analytical expressions of the NMR signals fitted to the recorded data, we can determine a generalized dispersion coefficient in the case of super dispersion. Using NMR velocimetry data collected in a homogeneous 30  $\mu\text{m}$  grain pack and  $10 < \text{Pe} < 35$ , we quantified the observed weak super dispersion in saturated conditions, and the strong super-dispersion observed during steady-state oil–water two phase flow.

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## 1. Introduction

Dispersion in porous media has been studied for a long time from breakthrough curves using a tracer [1]. Typically, one monitors at the outlet of a porous medium the spreading of a spike of tracer (a miscible fluid) injected at the inlet. In the simplest case (normal dispersion), the concentration vs. time curve is Gaussian and analyzed using an advection–dispersion equation (ADE) to obtain a dispersion coefficient  $D$ . It is well known that such approach is limited to homogeneous porous media. The Pulsed Field Gradient (PFG) NMR method is much more direct since the distribution of molecule displacements (propagator) is measured. Indeed the variance (or second moment) of this distribution is directly linked to the dispersion coefficient  $D$  without any assumption. This property has been used by many authors and results from both methods give comparable results (see [2] for a compilation of results), although NMR tend to give lower  $D$  values. This simple approach does not apply in porous media with a complex structure such as double porosity carbonates [3], or in two phase flows performed in homogeneous systems [4]. Here,  $D$  varies in time and space. In such cases, models containing more parameters need to be used in order to correctly reproduce the tracer displacement and as a consequence, more experimental information is necessary. For tracer experiments, this implies that the space dependence of the concentration vs. time must be acquired, and

for NMR, the time dependence of propagators should be analyzed. For NMR, this time dependence is naturally examined and if the variance  $\sigma^2$  does not vary linearly with time,  $D$  will not be unique and depend on time. This means that we cannot characterize the porous medium with a unique dispersion coefficient.

In this work, we propose to extend the standard second moment NMR analysis and exploit all information contained in PFG-NMR experiments. Indeed, the second moment derived from the NMR signal only takes into account small wave numbers. Alternatively, fitting the propagator with Gaussian or non-Gaussian models is strongly affected by the way the Fourier transform is performed. Thus, in order to avoid these deficiencies the best way to simulate super-dispersion is to build a model predicting directly the PFG-NMR signal. This is indeed the case when using numerical methods such as CTRW stochastic models (see [1] for a general presentation) in which the details of the porous media are not represented. Instead the probability of a displacement is taken from various probability density functions designed to reproduce physical effects. For example, molecules may be trapped in non-flowing zones and this may be expressed as a larger probability of zero displacement compared to the Gaussian case. The approach presented here uses similar concepts without the need for numerical simulations.

## 2. Theory

The proposed model is very general and attempts to reproduce two important mechanisms: (i) the possibility for a molecule to be

\* Corresponding author. Tel.: +33 147526289.

E-mail address: [marc.fleury@ifpen.fr](mailto:marc.fleury@ifpen.fr) (M. Fleury).

temporarily trapped in non-flowing zones and (ii) the possibility for a molecule to travel large distances due to for example a highly contrasted velocity field. Hence, we reproduce deviations from the Gaussian case either by modifying the short or long displacement tails on both sides of the distribution. Empirical choices for representing these mechanisms were made: for the first mechanism, the well-known Mobile–Immobile concept is used [1], and for the second mechanism, the idea of Levy motions is exploited with the important advantage that it includes the Gaussian case. The model is called SMIM, an acronym for space fractional Mobile Immobile Model. It is not the purpose of this short document to give the tedious details of the theory presented elsewhere [5]. The complex PFG-NMR signal is given by the following analytical expressions:

$$E(q, \Delta t) = \langle e^{-iq\Delta x} \rangle = (F_- + GM)e^{r_- \Delta t} - (F_+ + GM)e^{r_+ \Delta t} \quad (1)$$

where:

$$F_{\pm} = \frac{\eta}{K+1} \frac{A_{\pm}}{r_{\pm}} \quad G = \frac{K\eta}{K+1} \frac{1}{\sqrt{\Delta}} \quad M = e^{-\omega(K+1)\tau_1}$$

$$\eta = iqv + D|q|^{\alpha} \left[ 1 + \tan \frac{\pi\alpha}{2} \text{sign}(q) \right]$$

$$2r_{\pm} = -(\eta + \omega(K+1)) \pm \sqrt{\Delta}$$

$$A_{\pm} = \frac{\omega(K+1) - \eta}{2\sqrt{\Delta}} \pm \frac{1}{2}$$

$$\Delta = \eta^2 + 2\eta\omega(K-1) + \omega^2(K+1)^2$$

where  $q$  is the NMR wave number ( $q = \gamma\delta g$ , product of the gyromagnetic ratio, pulse length and amplitude respectively). The model has

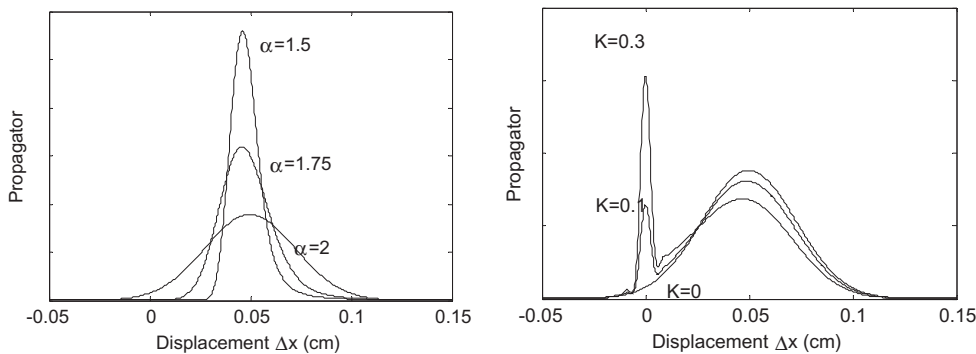
5 parameters  $D$ ,  $\alpha$ ,  $K$ ,  $\omega$ ,  $v$  and an auxiliary parameter  $M$  with the following significance:

- $D$ : generalized dispersion coefficient [ $\text{m}^{\alpha}/\text{s}$ ],
- $\alpha$ : stability exponent of the Levy distribution,
- $K$ : ratio of average immobile to mobile times,
- $\omega$ : parameter describing the distribution of immobile times (exponential function),
- $v$ : average velocity while moving (thus larger than the measured average velocity),
- $M$ : a parameter describing memory effects.

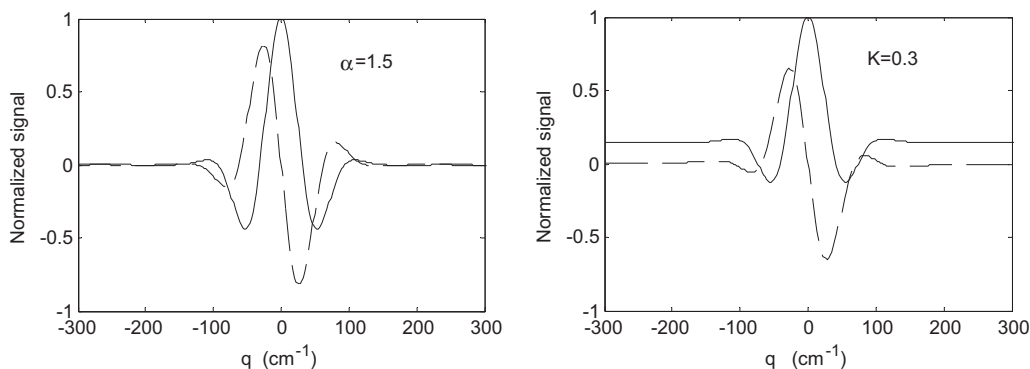
Since no further details are given about these parameters, it is also useful to present the partial differential equation describing tracer experiments to understand how the standard ADE equation is modified:

$$\frac{\partial C}{\partial t} + K\omega e^{-\omega t} * \frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} - D \frac{1}{\cos(\pi\alpha/2)} \frac{\partial^{\alpha} C}{\partial x^{\alpha}} \quad (2)$$

The parameter  $\alpha$  is present in the fractional derivative of order  $\alpha$  (definition given in [5]), and the trapping mechanism is identified by a supplementary term in the time derivative (the symbol \* indicates a convolution). When  $\alpha = 2$  and  $K = 0$ , Eq. (2) corresponds to the standard ADE. The possibility of reproducing a large variety of shapes with SMIM is shown in Fig. 1. We illustrate the two mechanisms mentioned above by setting first no immobile molecules ( $K = 0$ ) and varying  $\alpha$ . In this case, Fig. 2 we see gradually the formation of a tail at large displacements as  $\alpha$  decreases. In the second example, we set  $\alpha = 2$  and vary  $K$ , the ratio of average immobile to mobile times. We see a gradual increase of the peak at zero displacement. Varying  $\omega$  simultaneously would result in a larger or smaller width of this peak. If we combine both mechanisms, we modify simultaneously the large and small displacement tails. Note



**Fig. 1.** Example of propagators obtained from SMIM. Left: effect of  $\alpha$  with  $D = 0.5 \text{ cm}^2/\text{s}$ ,  $v = 0.1 \text{ cm/s}$  with no immobile time ( $K = 0$ ). Right: effect of  $K$  with  $D = 0.5 \text{ cm}^2/\text{s}$ ,  $\alpha = 2$ ,  $v = 0.1 \text{ cm/s}$ ,  $\omega = 1 \text{ s}^{-1}$ ,  $M = 0.5$ .



**Fig. 2.** Examples of complex NMR signals in  $q$  space, corresponding to 2 propagators shown in Fig. 1. Left:  $\alpha = 1.5$ ,  $D = 0.5 \text{ cm}^2/\text{s}$ ,  $v = 0.1 \text{ cm/s}$  ( $K = 0$ ). Right:  $K = 0.3$ ,  $D = 0.5 \text{ cm}^2/\text{s}$ ,  $\alpha = 2$ ,  $v = 0.1 \text{ cm/s}$ ,  $\omega = 1 \text{ s}^{-1}$ ,  $M = 0.5$ .

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