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Simulation of NMR-relaxation

Start with a pore radius distribution and a model of diffusion coupled pores

End with a relaxation time distribution



R₁₀ 12

3 x

10

cluster of pores

simulation of NMRrelaxation

using a corresponding electrical circuit



16x

Simulation of surface relaxation for one pore class and longitudinal magnetization





corresponding electrical circuit

 $R_{NMR} = \rho_1^{-1}/S$ $T = R C = (\rho_1^{-1}/S)V$ $= (\rho_1^{-1} r/3)$

relaxation time

Simulation of surface relaxation for one pore class and transverse magnetization





corresponding electrical circuit

 $\mathbf{R}_{\rm NMR} = \rho_2^{-1} / \mathbf{S}$ $T = R C = (\rho_2^{-1}/S)V$ $= (\rho_2^{-1} r/3)$ $\rho_2 = 5.85 \rho_1 (9.53/r)^{0.43}$

relaxation time

Simulation of surface relaxation and diffusion for two connected pores



$$P(t) = \sum_{i=1}^{n} P_i$$

relaxation curve of pore cluster

normed to $P_{t=0} = 1$

for isolated pores
$$P_i = V_i \exp\left(-\frac{t}{T_i}\right)$$

relative volumes V_i with $\sum_{i=1}^{n} V_i = 1$

 T_{i} is a function of pore radius r_{i}

for connected pores $P_{i} = \sum_{j=1}^{n} b_{ij} \exp\left(-\frac{t}{T_{j}}\right)$

$$\sum_{j=1} b_{ij} = V_i$$

The relaxation times T_j are common for all connected pores, however the coefficients b_{ij} are different.

Some b_{ij} may be negative.

relaxation curve of pore cluster from coefficients of connected pores

$$P(t) = \sum_{j=1}^{n} \left(\sum_{i=1}^{n} b_{ij}\right) \exp\left(-\frac{t}{T_{j}}\right)$$

analytical calculation of NMR relaxation by solving a system of linear differential equations

example for a cluster of three pore classes

A =



$$Y' = AY$$

$$P'_{1}$$

$$Y' = P'_{2}$$

$$P'_{3}$$

$$Y = P_{1} P_{2} P_{3}$$

$$\frac{\left(\left(R_{NMR,1}\right)^{-1}+11\left(R_{diff,1_{2}}\right)^{-1}\right)}{C_{1}} \qquad \frac{-11\left(R_{diff,1_{2}}\right)^{-1}}{C_{1}} \qquad 0 \\
\frac{-\left(R_{diff,1_{2}}\right)^{-1}}{C_{2}} \qquad \frac{\left(\left(R_{NMR,2}\right)^{-1}+\left(R_{diff,1_{2}}\right)^{-1}+16\left(R_{diff,2_{2}}\right)^{-1}\right)}{C_{2}} \qquad \frac{-16\left(R_{diff,2_{2}}\right)^{-1}}{C_{2}} \\
0 \qquad \frac{-\left(R_{diff,2_{2}}\right)^{-1}}{C_{3}} \qquad \frac{\left(\left(R_{NMR,2}\right)^{-1}+\left(R_{diff,2_{2}}\right)^{-1}\right)}{C_{3}} \qquad \frac{\left(\left(R_{NMR,3}\right)^{-1}+\left(R_{diff,2_{2}}\right)^{-1}\right)}{C_{3}} \\$$

$$R_{NMR,i} = (\rho S_i)^{-1} \qquad R_{diff,1_2} = D^{-1} l_{1_2} A_{cross,1_2}$$
$$R_{diff,2_3} = D^{-1} l_{2_3} A_{cross,2_3}$$





relaxation function of sub-cluster

sub-clusters











3 X V10 V11

16x







relaxation time distribution

transverse magnetization compared to longitudinal magnetization

