Electric Current Density Imaging of Chemical Reactions

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Introduction

Electric current density imaging (CDI) is a magnetic resonance imaging technique that images induced current density and conductivity distribution within a sample [1, 2]. Electric currents that flow through the sample change the magnetic field in the sample. The changed magnetic field B_c is added to the static magnetic field and causes a shift in the Larmor frequency $\omega_c = \gamma B_c$. The frequency shift is obtained by measuring the phase shift $\varphi_c = \omega_c T_c$, where T_c is total duration of applied electric currents. Once the magnetic field change B_c is known electric current density can be calculated using the Amper`s law $\boldsymbol{j} = 1/\mu_0 \boldsymbol{\nabla} \times \boldsymbol{B}_c$. In this study this technique is used for imaging the spatial variation of the ionic concentration during dissolving of a tablet [3]. Ion migration was modeled using the diffusion equation. For different acids diffusion constants were calculated by fitting experimental data to the theoretical model.

Methods

CDI experiments were performed on 100 MHz Bruker Biospec system equipped with micro-imaging accessories. Experiments were carried out in plexi-glass cell filled with 1% agar-agar gel. The cell contained two concentric cylinders. The inner cylinder with a diameter of 10 mm and 12 mm in length had electrodes on both ends, so that electric currents were flowing along the cylinder axis. The electrodes were connected to an amplifier with 220 V output voltage. The outer cylinder with a larger diameter (16 mm) was used as a reference and was also filled with 1% agar-agar gel, but no current was flowing through it. A cylindrical tablet with dimensions: diameter, 3 mm and height, 12 mm was placed in the center of the inner cylinder and data acquisition started. The dissolving processe followed by ion migration was monitored by CDI at regular time intervals of approximately 4 minutes until the tablet was completely dissolved and the current density was uniform through the inner cylinder. Experiments were done for citric, oxalic, maleic, and tartaric acids. Diffusion constants for these materials in 1% agar-agar gel were determined from CDI images.

Images of electric current density j_z in xy plane was calculated using the equation $j_z = 1/\mu_0 (\delta B_c^y/\delta x - \delta B_c^x/\delta y)$. In order to calculate the map of electric current density j_z, two maps of magnetic field change ($\delta B_c^y/\delta x$ and $\delta B_c^x/\delta y$) are needed. Normally, this would imply the sample rotation for 90° around the z axis. However, the samples in our experiments had cylindrical symmetry so that two acquired current phase shift maps, which are used to calculate corresponding magnetic field maps, were the same and therefore only one image was used to calculate electric current density j_z. The imaging parameters were: FOV = 25 mm, slice thickness 5 mm, TR = 600 ms, TE = 32 ms and T_c= 20 ms.

Results

Once the acid tablet was inserted into the 1% agar-agar gel, positive and negative ions started to separate and migrate away from the tablet. The concentration of mobile ions changes gel conductivity and therefore reflects in CDI images. Current density images thus show a progression of tablet dissolution and ion migration (Fig. 1, left column), while no difference (except for the position of the tablet at the beginning of the experiment) is observed on conventional MRI images (Fig. 1, right column). The diffusion coefficient can be determined from the average signal intensity of CD-images acquired at different times after the beginning of the dissolution process (Figure 2).

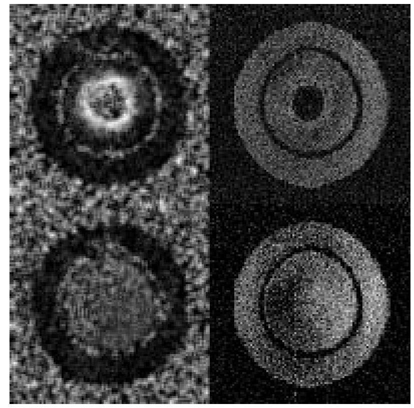

Figure 1: CDI (left column) and MRI (right column) of maleic acid at two different times (upper row: t=230 s, lower row: t=3200 s). The intensity of the CDI represents the concentration of positive and negative ions (black: no electric current, white: maximum electric current).

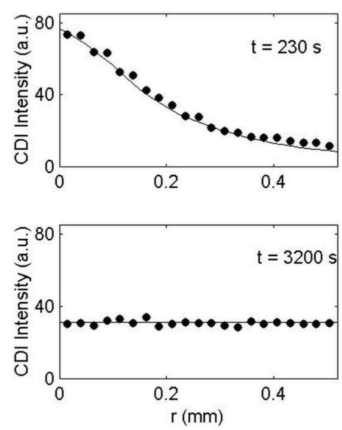

Figure 2: Average intensity of the CDI between the edge of the tablet before dissolving (r=0) and the edge of the inner cylinder (r=0.5 mm); circles: measured values, line: theoretical fit.

Discussion

CDI technique enables monitoring of spatial and temporal changes of conductivity. The potential use of this technique is for monitoring migration of ions through liquids and membranes. Thus, it can be used in pharmaceutical sciences where the dissolution of drugs from tablets, powders, and granules and distribution of drug molecules in tissues is important. These processes cannot be monitored by conventional MRI, since it can only show changes in the size of the tablet during dissolving, whereas CDI can detect also ion distribution around the tablet. CDI may be therefore important for better understanding of the transport of drug molecules in tissues.

References

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