

# Chemical Engineering Thesis Defense

Synthesis and Characterization of Amphiphilic molecules  
for their use in health care industry

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## abstract

Amphipathic molecules consist of hydrophilic and hydrophobic regions, which make them surface-active molecules. The uniqueness of these compounds results in inducing low surface tension and self-assembly of the molecules inside a solvent which have been exploited in personal care, oil industry and agriculture industry. Amphipathic molecules are also used in the health care industry as drug delivery systems and other bio-nanotechnology applications. In this thesis, a novel series of grafted siloxanes have been explored for their probable application in the health care industry. The siloxanes are grafted with poly(ethylene glycol) (PEG) and Quaternary ammonium salt (QUAT). The effects of varying 1) molar ratios of QUAT to PEG and 2) PEG chain length on contact angle, surface tension, critical micelle concentration (CMC), and micelle assembly properties were studied. In contact angle experiments, the hydrophilicity of grafted siloxanes increased by grafting PEG and QUAT. The amphiphilicity increases and CMC decreases as the PEG chain length shortens. Adding QUAT also reduces CMC. These trends were observed in surface tension and Isothermal Titration Calorimetry experiments. A change in self-assembly behavior was also observed in Dynamic Light Scattering experiments upon increasing the PEG chain length and its ratio relative to the quaternary ammonium in the siloxane polymer. These polymers have also been studied for their probable application as a sensitive  $^1\text{H}$  NMR spectroscopy indicator of tissue oxygenation ( $p\text{O}_2$ ) based on spectroscopic spin-lattice relaxometry. The proton imaging of siloxanes to map tissue oxygenation levels (PISTOL) technique is used to map  $T_1$  of siloxane polymer, which is correlated to dynamic changes in tissue  $p\text{O}_2$  at various locations by a linear relationship between  $p\text{O}_2$  and  $1/T_1$ . The  $T_1$ -weighted echo spin signals were observed in initial study of siloxanes using the PISTOL technique. The change in the ratio of QUAT to PEG and the varying chain length of PEG have a significant effect on the physical property characteristics of siloxane graft copolymers. The conclusions and observations of the present work serve as a benchmark study for further development of adaptive polymers and for the creation of integrated “nanoscale” probes for PISTOL oximetry and drug delivery.

June 28, 2018; 12 PM; ECA 219