

## **Novel Antimicrobial Waterborne Polyurethanes**

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Polyurethanes (PUs) are a versatile class of polymers used in a large scale of applications. They have been used as coatings for wood finishing, biomedical applications, glass fiber sizing, adhesives, automotive parts and finishes, gloves and other applications. The use of solvent based PUs is a source of increasing concern for health, safety and the environment, so there has been a strong preference for waterborne resins.

Barrier materials and coatings are used for the protection of structures and people. Current deficiencies include lack of antimicrobial effectiveness, lack of durability, and release of the agent into the environment. Environmental concerns stimulate the search for better coatings/films/fibers exhibiting low release of antimicrobial agents into the environment. Currently utilized materials do not meet the expected environmental regulations. This proposal focuses on the development of a new type of waterborne polyurethane, suitable for the above mentioned applications. The antimicrobial properties will result from incorporation of quaternary ammonium groups covalently bonded to the polymer backbone. The expected features of these polymers are a relatively high stability and good antimicrobial properties.

The work during this period involved the synthesis of a new quaternary ammonium compound and two families of PUs containing pendant carboxyl and quaternary ammonium groups that are incorporated as an enabling group in PU for producing dispersion in water. The polymer was dispersed in water and characterized.

### **1) Results**

**Quaternary Ammonium Salt (QAS) Preparation** monomers were synthesized at room temperature using water as a solvent.

### **Polyurethane (PU) Synthesis**

Two families of polyurethanes were synthesized by using two step condensation reaction. DMPA and quaternary ammonium salt were used as a chain extender. The final polymer was

dispersed in water. As a result, anionically stabilized micelles with a multiplicity of polyurethane and urea groups were produced.

### **Reaction Characterization**

During the PU reaction, NCO group formation was followed by FTIR instrument analysis. The isocyanate peak, observed at  $2270\text{ cm}^{-1}$ . While the reaction proceeded: N=C=O peak decreased and disappeared totally. As a result it can be concluded that polyurethane reaction took place. In addition the IR spectrum of QAS monomer was analyzed. The epoxide ring, which was observed in the spectra of the glycidyl phenyl ether, disappeared in IR spectra of the QAS.

$^{13}\text{C}$ -NMR spectra of the obtained polymers were taken with the use of the spectrometer Bruker AV-400 spectrometer, operating at 400 MHz Analysis was carried out in DMSO. Chemical structure of the synthesized quaternary ammonium salt was verified on the basis of  $^{13}\text{C}$ -NMR spectra.

### **Thermal Characterization**

Thermal transitions of both PUs were studied. The melting and crystallization transitions of the soft segment formed by the long diol were reported as  $20.70\text{ }^{\circ}\text{C}$ ,  $-2.59\text{ }^{\circ}\text{C}$ .

### **Particle Size Analysis**

Particle size distribution of the waterborne polyurethane (WBPU) dispersion was measured by dynamic-light scattering using a NICOMP<sup>TM</sup> 380 ZLS particle sizing system. The experiment was carried out at room temperature ( $25\text{ }^{\circ}\text{C}$ ), and the mean particle size and the size distribution were determined. The sample was first diluted with de-ionized water and the dispersion was homogenized before testing. The effect of water content, mixing time and mixing speed on particle size was studied. Moreover, the effect of water content on viscosity was examined.

### **Future Work**

During the following phase of this proposal, we will study:

- 1) The effect of changes to the ratio of DMPA (ionic content) and 1,4 BD on particle size distribution and viscosity of the emulsion.

- 2) Antibacterial behavior of the system will be studied by attaching quaternary ammonium compounds to the polymer backbone. Morphological and mechanical properties of the antibacterial dispersion will be studied.

### **Presentations**

- 1) “Waterborne Polyurethanes” Auad M.L, Demir B., Broughton R. 237<sup>th</sup> ACS National Meeting, Salt Lake City Utah, United States, March 22-26, 2009.