

CHEE 897 Student Seminar Day 2011

Thursday, December 8th Room 215

10:00am

NAME: David Hyslop

TITLE: Functionalized Nitroxyls for Enhanced Control of Free Radical Crosslinking of Peroxide Curable Materials

ABSTRACT:

Peroxide-curable materials form crosslinks in the presence of high energy free radicals through macroradical combination or propagating chain sequences of polymer-bound unsaturation. Antioxidants are commonly added in the early stages of a cure to delay the onset of crosslinking to allow for processing and moulding of the melt before it sets, commonly known as 'scorch protection'. These inhibiting additives consume initiating species, decreasing the overall efficiency of peroxide cures and potentially contribute to the presence of unbound leechables in the final article. The work presented explores a series of functionalized, nitroxyl-based free radical species used as a means of providing excellent scorch protection and a clean cure without compromising initiator efficiency. The novelty of this approach relies on the rapid, irreversible trapping of intermediate macroradical species and subsequent polymerization of the newly grafted functionality to latently incorporate trapped polymer sites into the developing network.

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10:30am

NAME: Hadiseh Karimi

TITLE: Parameter Estimation in a Nylon 66 Degradation Model

ABSTRACT:

An improved kinetic model for thermal non-oxidative degradation of nylon 66 is proposed and parameters are estimated using experimental data. This model predicts the rates of undesirable reactions that can occur in the finishing stages of commercial nylon 66 production when water concentration is low (10 to 80 molMg⁻¹) and temperature is high (275 to 292C). High temperature and low water concentration are used to achieve high molecular weight and high polycondensation rate. The model accounts for all of the observed degradation products and describes the noticeable effect of melt-phase water concentration on thermal degradation. Maintaining sufficient water in the reacting mixture helps to reduce degradation. Estimability analysis and a mean-square error (MSE) criterion are used to select parameters and unknown initial conditions for estimation. Estimability analysis is used to rank parameters from most important to the least important, and the MSE criterion determines which parameters should be estimated to provide the best predictions using the available data. The MSE criterion determined that 43 out of 56 parameters should be estimated with remaining parameters held at their nominal values. The model is a useful tool for predicting gelation and the rate and extent of thermal degradation under process conditions of commercial interest.

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11:00am

NAME: Siqing Yue

TITLE: The role of members of a biofilm consortium in the biodegradation of naphthenic acids in an immobilized soil bioreactor

ABSTRACT:

Every barrel of oil produced from the Alberta tar sands by caustic hot water extraction requires 3-5 barrels of fresh water, and thus results in large quantities of oil sand process wastewaters (OSPW) which must be treated prior to discharge. The treatment of OSPW has become a critical environmental issue because of its toxicity which is thought to be primarily due to naphthenic acids (NAs). Biofilms in two immobilized soil bioreactors (ISBRs) in series were developed to degrade and/or detoxify the OSPW. A 16S rDNA clone library of the inoculum used to develop the biofilm was constructed and can be used in combination with denaturing gradient gel electrophoresis (DGGE) to monitor the change in the bacterial population with the change in operating conditions. This study revealed that both Nitrosomonas and Rhodanobacter are predominant groups in the reactor. In a separate study, Rhodanobacter and 4 other isolates were obtained on agar plates containing extracted NAs as the sole carbon source from the second ISBR. All isolates including Rhodanobacter completely degraded 1 g/L cyclohexanecarboxylic acid but did not grow on as little as 30 mg/L Merichem NAs. It would appear that Rhodanobacter and the other isolates may be actively involved in the degradation of the OSPW and may play a key role in microbial community in the ISBRs.

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11:30am

NAME: Karthik Vikram Siva Shanmugam

TITLE: Fundamentals of Bis-maleimide Cure Chemistry

ABSTRACT:

Radical-mediated polymer modifications are robust and inexpensive methods of transforming commodity elastomers and thermoplastics into thermoset articles. Although coagent technologies for improving cross-linking yields are well-established, commercial development has evolved faster than our understanding of underlying chemical principles. This work aims to develop an understanding of a bis-maleimide based coagent system.

Rheological studies of cis-polybutadiene and LLDPE cure dynamics and yields are augmented with model compound studies to build a mechanistic understanding of these systems. NMR and MS analysis of the products derived from reacting N-phenylmaleimide with cyclooctane indicates that C-H bond addition is the primary means of cross-linking in LLDPE. Similar studies of N-phenylmaleimide reactions with cis-cyclooctene revealed an alternating copolymerization mechanism for polybutadiene + bis-maleimide cures.