CHEE 897 Student Seminar Day 2011

Thursday, September 15th Room 215

10:00am

NAME: Ying Zhang

TITLE: Foaming Behaviour of Coagent Modified Polypropylene

ABSTRACT:

Reactive modification of linear PP by radical mediated grafting in the melt state is investigated as a means of increasing the melt strength of linear PP to improve its foam processing. Tri-functional coagents, trimethylolpropane trimethacrylate (TMPTMA) and triallyl trimesate (TAM) are used to introduce long chain branching to a linear PP homopolymer. Rheological characterization as well as GPC measurement is conducted to relate the rheological properties to the modified PP chain architecture. The foaming behaviour of modified and original PP is investigated using a batch foaming apparatus with N2 as a blowing agent. It has been found that the investigated modification route is capable of introducing long chain branching into linear PP, which results in improved foaming behavior.

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Thursday, September 15th Room 215

10:30am

NAME: Rajesh Parmar

TITLE: A comprehensive kinetic and mechanistic study of gas phase reactions during autothermal reforming of diesel surrogate.

ABSTRACT:

The current research falls under umbrella of overall objective of Solid Oxide Fuel Cell (SOFC) Network, Canada to design 1 KW diesel fed SOFC pilot system. One of the sub-themes of the Network is to develop a kinetic model for optimum design of diesel reformer. The present discussion focuses on gas phase kinetic study during autothermal reforming of diesel surrogate (i.e. Tetradecane).

A 3-level factorial design experimental study for diesel surrogate reforming on Rh-Pyrochlore catalyst revealed that gas phase kinetics is very important and a suitable reaction mechanism to get the kinetics of gas phase reactions is essential in determining the reactant species reaching catalyst bed so that the mechanism of the surface reactions can be deconvoluted from the overall rate measurements. A complete packed bed reactor model is developed and temperature profile without reaction inside the reactor is validated against experimental data. A reaction mechanism and kinetic model is generated using the Reaction Mechanism Generator (RMG) software. In this predictive approach, a kinetic model is generated a priori using an algorithm based on a set of reaction rules for different functional groups. These rules are derived from kinetic and thermodynamic data determined using quantum chemistry and experimental results. The generated reaction mechanism has 7462 reactions and 478 species. Unfortunately it is difficult to handle complete momentum, heat and mass transfer with reactions in commercial software. Hence the model is simplified as plug flow reactor eliminating momentum transfer solution. An iterative approach is used in which temperature profile is solved in finite element solver and reaction rate and volumetric heat production profile is solved in CHEMKIN solver (that can handle such a large system of ODEs for plug flow reactor effectively). Iterations are repeated until no more change in temperature profile between last two iterations is obtained. The concentration profile at the outlet of reactor is validated against experimental data for various operating conditions.

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Thursday, September 15th Room 215

11:00am

NAME: Scott Amiss

TITLE: TBA

ABSTRACT:

TBA

CHEE 897 Student Seminar Day 2011

Thursday, September 15th Room 215

11:30am

NAME: Aida Khosravi

TITLE: Catalyst coating, reactor design, and catalytic activity test system set up for a high performance diesel fuel processor development

ABSTRACT:

Fundamental changes in society's energy systems are required to meet the efficiency and reliability improvement needed in terms of resources limitations. Lower rates of energy consumption, reduction in pollutants, and CO2 emission could be met by the use of fuel cells in electric power plants and transportation systems. Fuel cells require hydrogen for their operation; consequently numerous technologies are under investigation for generation and storage of hydrogen. Fuel processing is a technical term for a chemical conversion and conditioning of hydrocarbon fuels into a rich hydrogen gas stream that can be fed into fuel cells.

Reforming of diesel fuel is very attractive for hydrogen production due to high energy density and existing infrastructure for distribution; however the complexity and high heat input demand of the reforming reaction for diesel creates a significant challenge. Micro-structured reactors have been considered a promising option in recent years due to their high heat transfer capabilities that utilize the full potential of the catalysts for highly endothermic reactions and avoid hot spots formation for exothermic reactions. This work introduces a new design of metal plate reactor that allows repeatable estimation of the activity of catalyst coatings being developed for micro-structured reactors. The simple geometry provides a relatively easy analysis to extract kinetic parameters for reactor design purposes.

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Thursday, September 15th Room 215

12:00am

NAME: Abdulrahman Ashri

TITLE: TBA

ABSTRACT:

TBA