SIMULATION OF PROPYLENE POLYMERIZATION IN LABORATORY REACTORS

Ahmad Al-Shaiban, Joao Soares;

Department of Chemical Engineering, University of Waterloo, 200 University Av. W., Waterloo, ON, Canada, N2L 3G1

INTRODUCTION:

A model for propylene polymerization using a single-site catalyst with two states was developed to account for regio- and stereoregularity in polypropylene. The 1-2 and 2-1 insertions are modeled as two different monomer insertions, where M_1 represents the regular 1-2 insertion and M_2 the irregular 2-1 insertion. Stereoregularity is regulated by the type of active site: C_1^* is a stereoregular site that produces isotactic polymer chains, and C_2^* is a non stereospecific site that produces atactic polymer chains. Population balances were developed for this model and the method of moments was used to predict molecular weight averages.

KINETIC MODEL:

Activation

$$C_1 + Al \xrightarrow{k_{a1}} P_0^1$$

$$C_2 + Al \xrightarrow{k_{a2}} P_0^2$$

$$P_0^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_0^1$$

Initiation

$$P_0^1 + M_1 \xrightarrow{k_{i11}} P_{1,1}^1$$

$$P_0^1 + M_2 \xrightarrow{k_{i12}} P_{1,2}^1$$

$$P_H^1 + M_1 \xrightarrow{k_{iH11}} P_{1,1}^1$$

$$P_H^1 + M_2 \xrightarrow{k_{iH12}} P_{1,2}^1$$

$$P_{1,1}^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_{1,1}^1$$

$$P_{1,2}^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_{1,2}^1$$

$$P_H^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_H^1$$

Propagation

$$P_{r,1}^1 + M_1 \xrightarrow{k_{p1,11}} P_{r+1,1}^1 \qquad P_{r,1}^2 + M_1 \xrightarrow{k_{p2,11}} P_{r+1,1}^2$$

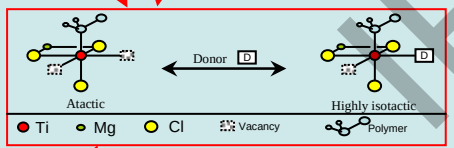
$$P_{r,1}^1 + M_2 \xrightarrow{k_{p1,12}} P_{r+1,2}^1 \qquad P_{r,1}^2 + M_2 \xrightarrow{k_{p2,12}} P_{r+1,2}^2$$

$$P_{r,2}^1 + M_1 \xrightarrow{k_{p1,21}} P_{r+1,1}^1 \qquad P_{r,2}^2 + M_1 \xrightarrow{k_{p2,21}} P_{r+1,1}^2$$

$$P_{r,2}^1 + M_2 \xrightarrow{k_{p1,22}} P_{r+1,2}^1 \qquad P_{r,2}^2 + M_2 \xrightarrow{k_{p2,22}} P_{r+1,2}^2$$

$$P_{r,1}^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_{r,1}^1$$

$$P_{r,2}^2 + Do \underset{k_{Do}^-}{\overset{k_{Do}^+}{\longleftrightarrow}} P_{r,2}^1$$



Termination

$$P_{r,1}^1 + H_2 \xrightarrow{k_{tH1,1}} P_H^1 + D_{r,1}^1$$

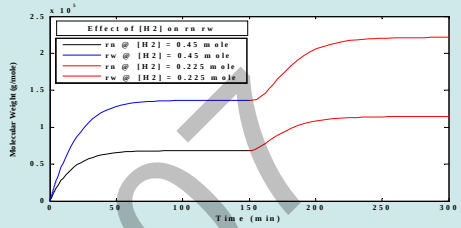
$$P_{r,2}^1 + H_2 \xrightarrow{k_{tH1,2}} P_H^1 + D_{r,2}^1$$

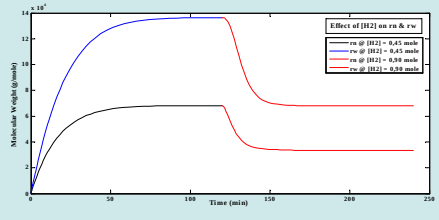
$$P_{r,1}^2 + H_2 \xrightarrow{k_{tH2,1}} P_H^2 + D_{r,1}^2$$

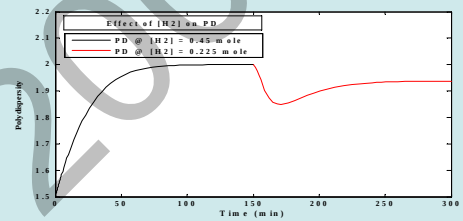
$$P_{r,2}^2 + H_2 \xrightarrow{k_{tH2,2}} P_H^2 + D_{r,2}^2$$

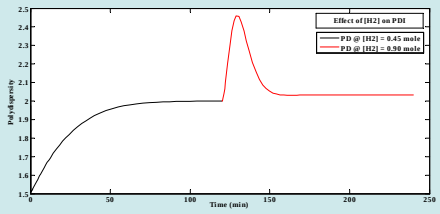
SIMULATION RESULTS:

Hydrogen Effect

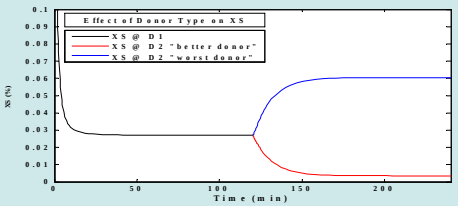


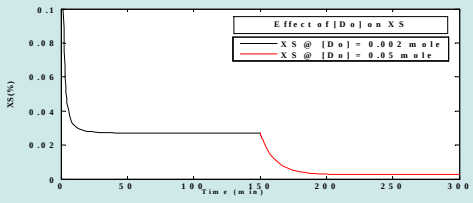






Donor Effect





CONCLUSIONS:

The following polymer properties can be simulated with our preliminary model: number and weight average molecular weight, polydispersity index, and soluble fraction. The model is also able to show the effect of different donors used in propylene polymerization. Moreover, the model is able to describe the regio and stereoregularity of these polymers. We plan to extend our model to account for the presence of several active site types and to validate it with literature values for propylene polymerization using different donors.

REFRENCES:

1. J. Soares, *Chemical Engineering Science* **56**, 4131 (2001)
2. J. Soares, T. McKenna, C. Cheng, Coordination polymerization. In *Polymer Reaction Engineering*, JM Asua (Ed.), Blackwell Publishing, in print. (2006)