Application of Genetic Algorithm for Identifying Ethylene/1-Olefin Copolymerization Conditions from Molecular Weight and Chemical Composition Distribution.

Uthane Nanthapoolsub, **Siripon Anantawaraskul**

Department of Chemical Engineering, Faculty of Engineering, Kasetsart University (Thailand)

The relationships between polymerization conditions and resulting chain microstructures were very important information for controlling the chain microstructures and final properties of polymers. Several approaches can be used to model polymerization kinetic and describe how each polymerization condition affects chain microstructures. To solve the inverse problem of determining appropriate polymerization conditions to tailor-make chain microstructures is, however, a rather complicated problem.

Previous works on such attempt were found that specifying only average chain microstructural information (e.g., average molecular weight, average comonomer content, polydispersity index) could easily lead to multiple solution problems. Recently, the information on 3D molecular weight and comonomer composition distribution (3D MWD/CCD) can be accessed more easily due to the commercialization of 3D TREF/GPC cross fractionation system. This abundance of information could provide the opportunity for solving this complicated problem. Genetic algorithm (GA), one of the efficient algorithms to provide global search in a large scale, was applied in this work as an optimization tool.

In this work, a genetic algorithm is used to perform global search to determine appropriate polymerization conditions from 3D molecular weight and chemical composition distribution. A series of the model data of a known ethylene/1-butene copolymerization with multiple-site-type catalytic system were used to validate the proposed method. The results showed that GA can be adequately used to identify the copolymerization conditions of ethylene and 1-butene from given 3D MWD/CCD information.

References:

1. J. B. P. Soares, Chem. Eng. Sci., 2001, 56, 4131.
2. B. Kou, K. B. McAuley, C. C. Hsu, D. W. Bacon, K. Z. Yao, Ind. Eng. Chem. Res., 2005, 44, 2428.
3. H. Hatzantonis, H. Yiannoulakis, A. Yiagopoulos, C. Kiparissides, Chem. Eng. Sci., 2000, 55, 3237.
4. T. Xie, K. B. McAuley, J. C. C. Hsu, D. W. Bacon, AIChE Journal, 1995, 41, 1251.