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Application of Genetic Algorithm to Optimize the Composition of Cu-Zn-Al-Sc Oxide Catalyst for Methanol Synthesis

<u>Tetsuo UMEGAKI</u>¹⁾, <u>Kohji OMATA</u>¹⁾, <u>Gunji ISHIGURO</u>¹⁾, <u>Yuhsuke WATANABE</u>¹⁾ and Muneyoshi YAMADA¹⁾

1) Dept. of Applied Chemistry, Graduate School of Engineering, Tohoku University (Received: October 4, 2002)

A genetic algorithm (GA), which is based on the theory of biological evolution, was applied to optimize the composition of Cu-Zn-Al-Sc oxide catalyst for methanol synthesis to identify high performance catalysts faster and more effectively. Using our own GA program where the activities from experiments were used as the fitness, we could almost optimize the composition by the fifth generation. The catalyst with maximum activity at the fifth generation had higher Cu/Zn ratio than conventional catalysts. The GA is a powerful tool to optimize catalyst composition.

Keywords: Genetic algorithm, Catalyst optimization, Combinatorial chemistry, Mixed oxide catalyst, Methanol synthesis, High throughput screening

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