**The Mechanism of Ethylene Dimerization in the Alphabutol Process and the Effects of Anti-Fouling Agents**

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The mechanism for ethylene dimerization to 1-butene in the Alphabutol Process is determined with the aid of density functional theory (DFT) to involve a complex catalyst mixture, the result of ligand exchange and hemi-labile coordination between titanium tetraalkoxide, trialkylaluminum, tetrahydrofuran (THF), and recently developed anti-fouling agents (AFAs) based on oligo(ethylene glycol). Previous theoretical studies have ignored the effects of THF, a key additive in industrial practice, and incorrectly predicted poor 1-butene selectivity. In this work, THF is shown to contribute to rate-determining barriers, and an inner-sphere beta-hydride transfer transition state is discovered to properly predict high 1-butene selectivity. The role of the conformationally complex and hemi-labile AFAs is explored with conformer-rotamer ensemble sorting tool (CREST), and the resulting DFT models correctly predict that AFAs lead to higher catalyst activity and 1-butene selectivity.

**Note to Essam, Katya, and other Aramco Americas reviewers:** It is known that Saudi Aramco has patented oligo(ethylene glycol) anti-fouling agents ( US Pat. No. 2017/0197892 ) to increase catalyst activity and 1-butene selectivity for the Alphabutol process. This abstract and the presentation would propose a mechanism for why the AFAs work. No novel chemicals would be suggested in the presentation.