Understanding Acid-Metal Balance in Paraffin Isomerization Using Multi-component Model Compound Probe Reactions

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Introduction
Single component model compound reactions have been invaluable in establishing acidity differences and metal-acid balance for many different catalytic reactions in fuels, lubes and chemicals processing due to its simple and analyzable products [1]. Spurred by improved molecular level understanding and analyses of real feeds, we believed that multi-component model compound studies would provide more valuable insights between the molecular feed species and the catalyst nanostructure and represented an important evolution in this approach to understanding reaction chemistry networks. This study will demonstrate the effectiveness of the new multi-component model compound feeds in evaluation of metal-acid shape selective catalysts and further reveal the bi-functional HI mechanism [2,3] under various feeds.

Materials and Methods
The model feeds were designed to simulate the real refining feed composition. For example, the four component model feed consisted of 60% n-hexadecane (a normal paraffin to track isomerization), 30% 2,4,10,14-tetramethylpentadecane (an isoparaffin to monitor the cracking), 5% 1-phenyloctane and 5% isopropylnaphthalene (long side-chain and branched side-chain aromatics respectively to reveal dealkylation and aromatic saturation).

The catalytic studies were performed using a continuous catalytic testing unit composed of a liquid feed system with an ISCO syringe pump, a fixed-bed tubular reactor with a three-zone furnace, liquid product collection, and an on-line GC for gas analysis.

Results and Discussion
The isomerization index derived from analysis of multi-component model compound system can predict the overall hydroisomerization catalyst performance by combining isomerization, cracking, dealkylation, and competitive adsorption into a single test parameter. This presentation will discuss how the use of this multi-component model compound reaction followed changes in hydroisomerization catalyst morphology and structure with such treatments as metal loading, zeolite/binder content and Si/Al ratio and how this understanding helped propel the improvement of bifunctional hydroisomerization catalyst. Figure 1 & Table 1 show the effectiveness of isomerization index in differentiating the HI catalyst performance. This indicated the establishment of optimal acid-metal balance based on feed composition will be critical for design of effective HI catalyst.

Conclusions
Fundamental studies using this new approach of multi-component model compound testing have successfully revealed the unique attributes of various HI catalysts for isomerization and provide understanding of “Non-Paraffin” chemistries affecting hydroisomerization. Utilizing the model compound reaction probes, our future research will focus identifying more active/selective HI catalysts as well as providing a stronger fundamentally based understanding of metal-acid balance and shape selectivity effects.

References