Catalyst Surface Chemistry Characterization Using Hexene Isomerization

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ABSTRACT

Heterogeneous catalysts can be used to speed or direct a reaction to produce desired products. Various properties of a catalyst, including surface chemistry, need to be determined experimentally before a catalyst can be used. The purpose of this research was to find a reliable method to characterize the surface chemistry of catalysts. Here hexane isomerization was used. The results reveal a clear distribution of products in the exit gases in the experimental situation. This research has provided a reliable method of finding the surface acidity of a catalyst.

INTRODUCTION

Heterogeneous catalysts are used in numerous chemical processes. These catalysts can be used to speed or direct a reaction to produce desired products. Various properties of a catalyst such as pore size, composition, and surface chemistry determine how it behaves in a reaction. Before a catalyst is used its properties need to be determined, so it can then be applied to the appropriate processes. Pore size and composition of a catalyst are determined during the manufacturing process and the catalyst is made to fit these specifications. The acidity of a catalyst is sometimes difficult to determine because it is influenced many factors. The surface chemistry of a catalyst should be found experimentally.

Catalysts can be used to remove organic compounds from water, convert carbon monoxide to less harmful gases, or to produce products such as maleic anhydride from n-butane. However, it is important to know the surface chemistry of a catalyst. If the wrong catalyst is used in a process it will not promote the desired reactions. Thus, knowing the surface chemistry of a catalyst allows engineers to determine what kinds of processes it can be used for.

The catalysts used for the processes mentioned above are all heterogeneous catalysts, but the surface chemistry of the catalysts varies. For example, Brita® water filters contain an activated carbon catalyst that is used to remove organic compounds and flavors from water. On the other hand, mufflers use a platinum based catalyst to reduce carbon monoxide emission by converting it to carbon dioxide. Vanadium Phosphorous Oxide (VPO) catalyst is used to convert n-butane to maleic anhydride. The activity of this catalyst favors production of maleic anhydride over combustion of the n-butane or production of aldehydes. The catalysts used for these processes are not interchangeable. The compositions and supports for the catalyst are different and this leads to very different surface chemistries.

The purpose of this research was to find a reliable method to characterize the surface chemistry of catalysts. The technique used in this experiment to determine the surface chemistry of the catalyst is hexene isomerization. Hexene is a six-carbon chain that contains one double bond. Rearrangement of the substrates on the chain and double bond migration are dependent on

acidity. The strength of an acid can cause double bond migration or rearrangements of the substrates on a hexene molecule.

EXPERIMENTAL DESIGN

Catalysts. Catalysts were prepared by Pacific Northwest National Laboratory (PNNL). Information regarding these catalysts is proprietary, so no information or results for the catalyst will be provided below.

Procedure. A 1-gram sample of the catalyst was loaded into a plug-flow reactor constructed of fused quartz (3/8 in I.D.). The catalyst was loaded between two pieces of quartz wool. A thermocouple was placed at the center of the catalyst bed so the bed temperature could be monitored. The reactor was placed in a tubular furnace and heated at 350oC for three hours while helium gas was passed over the catalyst at a rate of 13 (ml/min) (Logie, et al. 2000). Once the three-hour heating period was over a syringe pump was activated that contained 2-methyl-2-pentene (2M2P). The 2M2P was vaporized in a preheating line before it reached the reactor. The total volumetric flowrate was (19 ml/min) with the addition of the 2M2P.

Data Analysis. The gaseous products from this process were fed to an inline gas chromatograph to obtain the distribution of the product gases. The GC was calibrated to detect 2M2P, 4-methyl-2-pentene (4M2P), 3-methyl-2-pentene (3M2P), 2,3-dimethyl-2-butene (2,3-DMB-2). The readings from the GC were used to find the composition of the exist gas. These compositions were used to calculate the conversion of 2M2P and selectivities for the product gases. Weak acids cause the 2M2P to isomerize to 4M2P, strong acids yield 3M2P, and stronger acids favor isomerization to (2,3-DMB-2) (Natal-Santiago, et al. 1999). The surface chemistry of the catalyst could be determined using this information and the distribution of the produced gases.

RESULTS AND CONCLUSION

The technique described above for finding the surface chemistry of a catalyst was successful in these experiments. There was a clear distribution of products in the exit gases that could be used to find the conversion of 2M2P and selectivities for the products. These conversions and selectivities revealed the surface chemistry of the catalyst. This research is on-going and the results are reported to PNNL. PNNL has the information regarding the catalyst and may use the results to identify practical applications for the catalyst.

This research has provided a reliable method to find the surface acidity of a catalyst. The process used to complete this research is simple and non-hazardous. It can be carried out in any research facility with minimal capital investment. The chemicals are inexpensive and readily available for most chemical manufacturers.

Mass transfer and operating conditions heavily influenced these results. If the pore size of a catalyst is too small the hexene cannot diffuse into the catalyst and the product distributions will not be representative of chemistry of the catalyst. Additionally, it is important that the reaction conditions are optimal for isomerization. If temperatures are too high the hexene may crack. If the temperature is too low, the reaction will not take place.

REFERENCES

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