FINAL SCIENTIFIC/TECHNICAL REPORT

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Project Title: Advances in Process Intensification through Multifunctional Reactor Engineering

Recipient: Chemical Research and Licensing
10100 Bay Area Blvd.
Pasadena, TX 77507

Award Number: DE-FC36-04GO14152

Partners: Sandia National Laboratories, Lummus Technology (Division of CB&I)

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Executive Summary

This project was designed to advance the art of process intensification leading to a new generation of multifunctional chemical reactors utilizing pulse flow. Experimental testing was performed in order to fully characterize the hydrodynamic operating regimes associated with pulse flow for implementation in commercial applications.

Sandia National Laboratories (SNL) operated a pilot-scale multifunctional reactor experiment for operation with and investigation of pulse flow operation. Validation-quality data sets of the fluid dynamics, heat and mass transfer, and chemical kinetics were acquired and shared with Chemical Research and Licensing (CR&L). Experiments in a two-phase air-water system examined the effects of bead diameter in the packing, and viscosity. Pressure signals were used to detect pulsing. Three-phase experiments used immiscible organic and aqueous liquids, and air or nitrogen as the gas phase. Hydrodynamic studies of flow regimes and holdup were performed for different types of packing, and mass transfer measurements were performed for a woven packing. These studies substantiated the improvements in mass transfer anticipated for pulse flow in multifunctional reactors for the acid-catalyzed C4 paraffin/olefin alkylation process.

CR&L developed packings for this alkylation process, utilizing their alkylation process pilot facilities in Pasadena, TX. These packings were evaluated in the pilot-scale multifunctional reactor experiments established by Sandia to develop a more fundamental understanding of their role in process intensification.

Lummus utilized the alkylation technology developed by CR&L to design and optimize the full commercial process utilizing multifunctional reactors containing the packings developed by CR&L and evaluated by Sandia.

This hydrodynamic information has been developed for multifunctional chemical reactors utilizing pulse flow, for the acid-catalyzed C4 paraffin/olefin alkylation process, and is now accessible for use in other technologies.

Technical Achievements vs Expectations:

Hydrodynamic testing at SNL was completed as planned. However, initial plans included the evaluation of multiple CR&L packings at SNL to correlate the mass transfer characteristics of the packing with their physical properties. These correlations would have been used to optimize packing characteristics. Performance improvement would then have been verified through testing in the Pasadena facilities.

The three-phase testing at Sandia described above included chemical reaction as an indicator of mass transfer. The reaction selected proved difficult to monitor utilizing commercial chemicals, which delayed the implementation of these tests, limiting the quality and quantity of results mass transfer testing which could be completed. Thus although the improved performance of packings in pulse flow was confirmed, full optimization of packings was not achieved.

As expected, the studies substantiated the improvements in mass transfer anticipated for pulse flow in multifunctional reactors for gasoline alkylation.

Commercial Achievements vs Expectations

The apparent opportunity to implement process intensification using multifunctional chemical reactors to enhance inter-phase transport has been sulfuric-acid-catalyzed C4 paraffin/olefin

alkylation. Due to federal and state regulation of the sulfur content in gasoline in 2003, the United States was expected to require an additional 200 to 300 kbpd of alkylation product over the next five to ten years. Alternative technologies to manufacture alkylate faced emissions problems, redirecting industry to focus on process intensification strategies.

The economic benefits of the project were based on the continued expansion of the US economy projected in 2003/4 when the project was approved. US gasoline consumption was projected by DOE to expand beyond the volumes which could be provided using US refining capacity and the use of ethanol mandated by the Renewable Fuels Supply mandate (RFS1), then in place. Alkylate was needed to replace both the volume and octane value of MTBE which had been removed from gasoline, and offset the Reid Vapor Pressure (RVP) increase associated with ethanol.

Since that time ethanol mandates have been expanded (RFS2), and gasoline consumption has been reduced by a contraction in US economic activity, and a shift toward distillate fuels to gain fuel economy. Waivers for increased RVP gasoline also appear to be more acceptable as mandated levels of ethanol use have increased. Surplus refining capacity as well as ethanol usage increases have made it possible for refiners to meet fuel demand and quality requirements without the addition of alkylation capacity. Thus, the projected economic benefit for the US has not occurred, and is no longer expected to occur.

The CDTECH (CR&L and Lummus Technology, now both wholly owned by CB&I), alkylation technology has been selected for a new alkylation facility in the United States, using the CR&L developed packings. Because of the factors discussed above, the project has not been constructed. However, this technology continues to be offered for licensing throughout the world.

PROJECT DESCRIPTION AND REPORT

An Executive Summary and the detailed description of the program carried out at the Sandia National Laboratory is reported in Sandia Report SAND 2011-0673, “Advances in Process Intensification through Multifunctional Reactor Engineering”, printed in February 2011.
The Sandia Report has been provided to the DOE and is intended to be part of this report.