SAND2012-1701P

Sandia National Laboratories

Project Accomplishment Summary

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Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation
Albuquerque, New Mexico

PROJECT ACCOMPLISHMENTS SUMMARY

Cooperative Research and Development Agreement (#1689.00)

between **Sandia National Labs** and Catalytic Distillation Technologies

Note: This Project Accomplishments Summary will serve to meet the requirements for a final abstract and final report as specified in Article XI of the CRADA.

Title: Advances in Process Intensification through Multifunctional Reactor Engineering

Final Abstract:

This project was designed to advance the art of process intensification leading to a new generation of multifunctional chemical reactors. Experimental testing was performed in order to fully characterize the hydrodynamic operating regimes critical to process intensification and implementation in commercial applications. Physics of the heat and mass transfer and chemical kinetics and how these processes are ultimately scaled were investigated. Specifically, we progressed the knowledge and tools required to scale a multifunctional reactor for acid-catalyzed C4 paraffin/olefin alkylation to industrial dimensions. Understanding such process intensification strategies is crucial to improving the energy efficiency and profitability of multifunctional reactors, resulting in a projected energy savings of 100 trillion BTU/yr by 2020 and a substantial reduction in the accompanying emissions.

Background:

The multidiscipline, cooperative partnership between industry and government laboratories was formed to utilize the scientific and engineering expertise required to meet the short-term horizons of this ambitious program. Commercial reactors that enhance inter-phase transport via process intensification strategies would improve the energy savings and efficiency of sulfuric-acid-catalyzed C4 paraffin/olefin alkylation. Due to federal and state regulation of the sulfur content in gasoline, the United States was expected to require an additional 200 to 300 kbpd of alkylates over the next five to ten years. Alternative alkylate-producing processes face emissions problems, redirecting industry to focus on process intensification strategies. Currently, no commercial reactors have been designed to implement such strategies. Those reactors that do utilize such strategies are over-designed, resulting in less than ideal operating efficiencies. Characteristics of the hydrodynamic regimes comprising the most effective process intensification strategies lack fundamental scientific understanding. This knowledge is crucial for scaling up to industrial dimensions, process optimization, and commercialization. Our partnership seeks to gain scientific knowledge and engineering experience that will result in a new generation of multifunctional reactors designed for the most efficient of process intensification strategies. Such new technologies are identified in "Technology Vision 2020: The Chemical Industry" to provide for new, emerging process chemistries and to validate multiphase flow models at large and small scales.

Description:

The role of Sandia National Laboratories in the partnership is to fabricate and operate a pilot-scale multifunctional reactor experiment for operation with and investigation of process intensification strategies. Validation-quality data sets of the fluid dynamics, heat and mass transfer, and chemical kinetics were acquired and shared with the industrial partner. Experiments in a two-phase air-water system examined the effects of changing bead diameter in the packing, changing viscosity, and detection of pulsing through

examination of pressure signals. 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 the woven packing. There are several roles of CR&L in this partnership. The first is to develop packings that are optimal for this alkylation process, utilizing their alkylation process pilot facilities in Pasadena, TX. These optimized packings were evaluated in the pilot-scale multifunctional reactor experiment established by Sandia to develop a more fundamental understanding of their role in process intensification. In addition, CR&L is working with the University of Texas Separations Research Program to establish empirical hydrodynamic scale-up data and mass transfer information for these packings. This information will be useful background for the anticipated evaluation of the Sandia-developed surrogate technology in the large-scale UTSRP testing facilities. ABB Lummus' role is to optimize the full alkylation process, integrating the process intensification technology developed by Sandia and CR&L.

Benefits to the Department of Energy:

As part of this work, a mass transfer measurement technique was implemented in the reactor vessel. This provided the data showing that control of flow regime allowed increase of mass transfer rates between the immiscible liquid phases by at least an order of magnitude. The mass transfer technique measures the rate of conversion of fluorescein diacetate in the organic liquid into sodium fluorescein in the aqueous liquid. The technique is going to be applied for an ongoing LDRD project on nuclear waste reprocessing using centrifugal contactors. For reasons to be discussed below, the anticipated expansion of alkylation capacity in the United States did not occur. However, the technology required for process intensification through multifunctional reactors has been significantly advanced, and is now accessible for use in other technologies.

Economic Impact:

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 the volumes and octane 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 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.

Project Status:

Completed

ADDITIONAL INFORMATION

Laboratory/Department of Energy Facility Point of Contact for Information on Project

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Company Size and Points of Contact

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During the execution of this project the partners in CDTECH (ABB Lummus and CR&L) had ownership changes. Both were acquired by Chicago Bridge and Iron, and are now parts of Lummus Technology, a division of CB&I. All individual roles and responsibilities were assumed by Lummus Technologies, and executed as had been committed. However subsequent retirements, changes in employment, and the completion of much of the alkylation technology development, have resulted in the elimination of several of the primary technical roles associated with this Project. Dr. Arvids Judzis, Jr., Director, Technology Development for Lummus Technology retains the responsibility for this Project and the overall alkylation technology.

CRADA Intellectual Property

None

Technology Commercialization

No commercialization

Project Examples

None provided

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Cooperative Research and Development Agreement (SC04/01689)
between **Sandia National Laboratories** and **Catalytic Distillation Technologies**

This summary has been approved for public release by Sandia and Catalytic Distillation Technologies

Sandia National Laboratories

By _____ 6/27/11
Timothy J. O'Hern — Date
Principal Investigator

Sandia National Laboratories

By _____ 6/23/2011
Manager — Date
WFO/CRADA Agreements

Catalytic Distillation Technologies

By _____ 07/06/2011
Title: Managing Director — Date

In order to expedite the process, if we do not receive your signed reply by 07/28/2011 we will assume your concurrence for the release of this document to the public.