Sustainable Chemistry, the Spinning Tube-in-Tube (STT®) Reactor and GREENSCOPE: Innovation and Industrial Partnerships

Introduction

The chemical industry faces environmental, social and health challenges that are common across all economic sectors. From worker exposure to toxic substances, to product design and use, to the cost and handling of waste disposal, the industry must overcome numerous complex hurdles to secure a more sustainable future.

To help address these hurdles, EPA researchers are generating new strategies and approaches to developing cleaner technologies for synthesizing commodity and specialty chemicals. An interdisciplinary group of EPA researchers and their industrial partners are exploring innovative, reactor technologies and benign substitutes for harsh chemicals, catalysts and solvents. Their research applies green chemistry principles and philosophies to the design of new chemical processes. Furthermore, they apply green engineering principles to process intensification, which strives for better efficiency and safety, and for developing faster and more accurate processes and optimization. They use sustainability indicators to measure their improvements to the processes and to gauge their progress.

Process Design, Intensification and Optimization Using Green Chemistry and Engineering

Through industrial partnerships, EPA scientists and engineers are facilitating the development and wider adoption of green approaches that can produce thousands of different chemicals. This EPA research influences process design by applying principles of green chemistry and engineering, such as using increased mixing to replace toxic solvents. EPA researchers and their industrial collaborators are working at the interface of chemistry and chemical engineering for faster implementation of new reaction strategies in the marketplace. One resulting strategy is the application of the Spinning Tube-in-Tube (STT®) reactor (4 Rivers Biofuels, Calvert City, KY).

Research to date has demonstrated the STT® reactor can perform reactions without the need for any chemical inputs other than the reactants. One reactor, with a reactor zone volume of 1.2mL, can fit on a six-foot table, and is capable of producing up to 12 tons of product per year, depending on the residence time of the reaction. This feature is a demonstration of green engineering since the size of a plant using STT® reactors is orders of magnitude smaller than that needed for conventional chemical manufacturing with room-sized reactor vessels, separation towers, filtering systems and pipelines.

The increased mixing in the STT® reactor, which is based on a two-dimensional fluid film that flows longitudinally, allows for enhanced mixing. This allows for increased mass transfer, resulting in reaction rates up to three orders of magnitude greater than a conventional reactor. With this increased mass transfer, the reactor also allows for increased conversions, product selectivity and yields, and decreased energy usage, costs, and exposure risks to workers.

For faster process optimization, EPA researchers are utilizing real-time monitoring to identify product distributions as a result of altering reaction conditions. The real-time analytical data allow EPA researchers to optimize reaction conditions to yield maximum results in hours as opposed to days.

As an example, the STT® reactor has demonstrated the solvent-free preparation of a number of high purity, commercially relevant epoxides with excellent conversions and throughput. Additionally, the reactor has accomplished the high throughput production of high purity imines from a wide variety of starting aldehyde/ketones and amines in quantities and purities that are impractical or impossible via standard batch reaction techniques. Using this reactor and a wide variety of starting materials, researchers have also completed the high throughput production of high purity imidazole derivatives, which may be used as ligands in organometallic chemistry.

Below, EPA researcher and branch chief Michael Gonzalez works with the STT® Magellan Reactor with Mettler-Toledo IC-45 React IR.

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In conjunction with industrial partners, EPA researchers using the STT® reactor have developed oxidation, hydrogenation and esterification reaction chemistries. The reactor has the potential to be applied to the pharmaceutical, industrial chemical, food additive, and fragrance sectors. As a result of these collaborations, the reactor technology and its application have been licensed by two companies that aim to build commercial-scale operations to produce their consumer products.

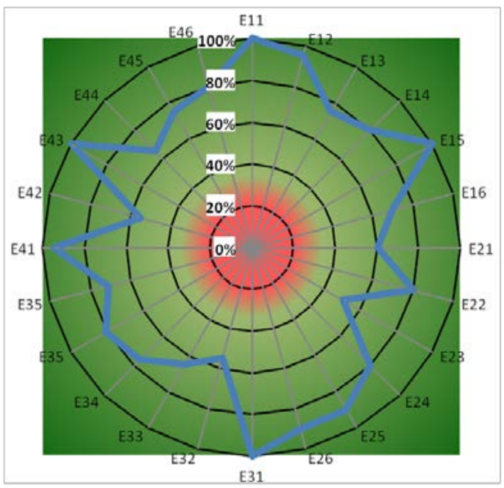
Reactor Modeling

With the advances in understanding the influence of reaction conditions in this novel reactor, efforts are on-going to model the STT® to fully understand the benefits observed, including increased reaction rates, yields and conversion. This modeling could lead to faster process optimization, will allow reaction conditions to be predicted, and will quantify results.

Sustainability Indicators

The GREENSCOPE or Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator research project team is creating a methodology that they will develop into a software tool that can assist researchers from academia, industry, and government agencies in designing more sustainable chemical processes. The sustainability of a chemical process can be evaluated in terms of four indicator areas: Environment, Efficiency, Energy and Economics, or the 4 E's. Within the 4 E's are 147 indicators that are representative of a chemical process. Each indicator is placed on a sustainability scale and provides a snapshot of the sustainability of the chemical process. To evaluate the environmental aspects of alternative chemistries or technologies, GREENSCOPE employs the Waste Reduction algorithm (Young and Cabezas, 1999). Efficiencies for chemical reactions are also reflected in indicators such as conversion and selectivity. GREENSCOPE has the ability to evaluate a new or existing process, perhaps one employing green chemistry principles on the laboratory scale, and to assess if it has a beneficial or negative effect on the overall sustainability of a chemical process or of a process that has been scaled up for industrial production.

Below, the indicators for a hypothetical process show measures (in blue) that fall between 0 and 100% of sustainability.



Industrial Partnerships

To address and tackle real-life challenges, apply sustainable solutions to these challenges, and partner with industry to infuse these technological solutions into the marketplace, EPA researchers have collaborated with many partners. The Spinning Tube-in-Tube (STT®) reactor research has led the EPA to collaborate with over 20 chemical companies, including two companies that took the results and research further. The work produced a potential patent application and spurred other chemical companies to collaborate with the EPA.

Since 2003, EPA researchers have collaborated with Kreido Laboratories (Camarillo, CA) through a Cooperative Research and Development Agreement involving the STT® reactor. Since 2009, the EPA has also been collaborating with the Four Rivers Energy Company to co-develop and advance the spinning tube-in-tube technology for chemical synthesis applications.

Companies that are interested and want to test the STT® technology for potential application can contact EPA researchers to arrange to use the needed facilities, staff and analytical equipment.

References

Smith, R. L. and Gonzalez, M. A. Methods for evaluating the sustainability of green processes. *Comp. Aided Chem. Eng.*, 2004, Vol. 18, 1135-1140.

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