CHEMICALS

Project Fact Sheet

Distillation Column Modeling Tools

Benefits

- Reduced CO_2 emissions
- Increased production capacity
- Improved column packing performance and operating conditions
- Reduced energy consumption and waste production

Applications

Approximately 40,000 distillation columns are presently in operation in the United States. The computational model that results from this research can be applied in the petroleum and petrochemical processing industries to optimize the performance of these distillation columns.

Advanced Computational and Experimental Techniques Will Optimize Distillation Column Operation

Distillation is a low thermal efficiency unit operation that currently consumes 4.8 quadrillion BTUs of energy—40% of the processing energy used in refining and continuous chemical processes. The multiphase gas/liquid flow patterns in distillation columns are complex, making them difficult to predict and control. Lack of understanding of the mass transfer and flow dynamics occurring between phases inside these devices is the primary barrier to improving their energy and process efficiencies.

New, advanced computational techniques to model distillation column operation could optimize separation processes and improve column packing design. To develop the proposed tools, advanced imaging techniques will be used to provide data for model development and to provide insight into distillation column operation. The resultant model will be validated at commercial scale to facilitate industry-wide acceptance and use. The commercialized software containing the model will calculate column design and operating parameters based on inputs of column size, packing configuration, feed conditions, and system physical properties. Using the model to optimize distillation column operations has the potential to save an estimated 53 trillion BTUs per year by 2020.

Distillation Columns

New computational tools optimize performance of distillation processes widely used in chemicals and petroleum refining.

Project Description

Goal: To develop a computational model based on first principles to optimize distillation column operation and design of column internals.

X-ray computed tomography will be used to image the flow characteristics within a column. After an extensive literature review, x-ray tomography was selected as the most promising technique for imaging vapor-liquid contactors. Laboratory- and pilot-scale fluidized beds, trickling filters, and stationary multiphase flow columns have been imaged using x-ray computed tomography. Initial tests have been completed using an existing imaging unit which indicated x-ray computed tomography has the potential to quantify the micro-scale hydraulics in a packed distillation column.

A variety of quantitative, predictive methods for dealing with multiphase flow systems are currently being developed. Lattice-Boltzmann methods are gaining rapid acceptance as the method of choice for simulation of complex systems. A lattice-free version of this method will be utilized in the proposed research.

Progress & Milestones

Project partners have completed initial imaging tests and are currently in the process of developing CFD models for simple contactor configurations.

Future work will center on completing the following milestones:

- Use x-ray imaging techniques to improve the understanding of the operation of a vapor-liquid contactor and to complete tests with packing test elements, simple commercial packings, and more complex commercial packing
- Develop, test, and validate computational model
- Perform pilot plant tests on operating distillation columns
- Develop commercialization plan.

Commercialization

The computational model will calculate column design and operating conditions based on inputs of column size, packing configuration, feed conditions, and system physical properties. It will be made accessible to all members of the petroleum and petrochemical processing industries through commercialization by Fluent. Fluent will work with Separations Research Program and Oak Ridge National Laboratory to integrate the new capabilities into its established, commercially available computational fluid dynamics software products. This will accomplish the technology transfer to industrial users, specifically enable packing vendors to design better packing materials, and enable optimization of existing distillation columns in the petroleum and chemical processing industries.

Project Partners

Fluent
Lebanon, NH

Oak Ridge National Laboratory
Oak Ridge, TN

University of Texas
Separation Research Program
Austin, TX

3D Imaging & Development, Inc.
Austin, TX

For additional information, please contact:

Dickson Ozokwelu
Office of Industrial Technologies
Phone: (202) 586-2501
Fax: (202) 586-9234
dickson.ozokwelu@ee.doe.gov

Please send any comments, questions, or suggestions to
webmaster.oit@ee.doe.gov

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Office of Industrial Technologies
Energy Efficiency
and Renewable Energy
U.S. Department of Energy
Washington, D.C. 20585

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