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Space-constrained purification of dimethyl ether through process intensification using semicontinuous dividing wall columns

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ABSTRACT

In this work, a distillation system is designed to purify dimethyl ether (DME) from its reaction by-products in the conversion of flare gas into a useful energy product. The distillation equipment has a size constraint for easy transportation, making process intensification the best strategy to efficiently separate the mixture. The process intensification distillation techniques explored include the dividing wall column (DWC) and a novel semicontinuous dividing wall column (S-DWC). The DWC and the S-DWC both purify DME to fuel grade purity along with producing high purity waste streams. An economic comparison is made between the two systems. The DWC is a cheaper method of producing DME however the purity of methanol, a reaction intermediate, is not as high as the S-DWC. Overall, this research shows that it is possible to purify DME and its reaction by-products in a 40-foot distillation column at a cost that is competitive with Diesel.

1. Introduction

1.1. Motivation

A major problem facing the energy industry of Alberta, Canada is the flaring and venting of solution gas from crude oil and crude bitumen production operations. Oil producers are making a great effort to capture these gasses and use them downstream, however it is not always economical to capture the solution gas and it is flared or vented to the atmosphere. According to the Alberta Energy Regulator, the energy industry captured 95.6% of solution gas produced in 2014, up from 95.3% in 2013 (Alberta Energy Regulator, 2016). Alberta's legislation on flaring, incineration and venting at upstream petroleum wells puts a daily limit on the amount of gas discharged at each extraction site and requires the implementation of gas conversion technologies if this limit is exceeded (Ellis, 2011). Low natural gas prices and high pipeline and compression costs challenge the economic viability of gas conservation (Alberta Energy Regulator, 2016). However, failing to generate useful energy from the flared gas misses the opportunity to offset electricity production from Diesel generators at the high cost of $0.40/kWh (Zubrin et al., 2016). As such, the solution is to convert the energy in the gas into a useful form using economical and small-scale technology. Due to recent tightening in Alberta's legislation (Ellis, 2011), there is a strong business case for the development of technologies that convert raw natural gas into a useful product, such as dimethyl ether.

Dimethyl ether (DME) is a new fuel that is becoming a popular alternative to traditional combustion fuels. DME is a non-toxic, non-corrosive, and non-carcinogenic odourless gas (Muller and Hubsch, 2000) and can be produced from a variety of feedstocks including natural gas and organic material. DME can be transported using the existing liquefied petroleum gas infrastructure and it can be used to power a Diesel engine with small modifications(California Environmental Protection Agency, 2015). A study by the Volvo Group comparing seven renewable fuels found DME as the leading fuel alternative in terms of cost, energy efficiency, land use, environmental impact, fuel potential, vehicle adaptation, and fuel infrastructure (AB Volvo, 2007). In comparison to Diesel, DME burns significantly cleaner, creating no sulphur oxide or particulate emissions and producing minimal nitrous oxides and carbon monoxide (Muller and Hubsch, 2000). One drawback of DME is that it has a

Abbreviations: ACCE, Aspen Capital Cost Estimator; CCA, capital cost allowance; CO_2, carbon dioxide; DME, dimethyl ether; DWC, dividing wall column; H_2O, water; MeOH, methanol; MV, middle vessel; PPDP, product and process design principles; S-DWC, semicontinuous dividing wall column; SwoMV, semicontinuous without middle vessel.

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density about 80% of diesel (at recommended storage conditions) and its specific energy content is about 70% of the energy content of Diesel; therefore, it is necessary to inject twice the fuel volume to yield the same power output as Diesel (California Environmental Protection Agency, 2015).

Dimethyl ether is commonly produced using one of two reaction pathways: a two-step and a one-step process. The two-step process first converts the syngas feedstock to methanol through the water-gas shift and methanol formation reactions. In a separate reactor, cleaned methanol is dehydrated to form DME. The product out of the DME reactor is a mixture of DME, unreacted methanol and water. This process is particularly useful since the production of methanol from natural gas is a mature industry and DME production can be added to existing methanol plants. On the other hand, the one-step process combines these reactions in one reactor and produces DME directly from syngas, with methanol being a reaction intermediate. In the single reactor, the water produced in the dehydration step helps drive the water-gas shift reaction forward, resulting in a higher conversion rate than the two-step process. Since there is no intermediate clean-up of methanol, the product out of the one-step reactor is a mixture of four components: DME, methanol, water and carbon dioxide (California Environmental Protection Agency, 2015).

1.2. Background

Process intensification is the drastic reduction in size, energy usage or waste production from a chemical plant and is used to improve the overall efficiency of industrial processes (Stankiewicz and Moulijn, 2000). Lately, these improvements are more easily developed because of recent advancements in computational speed making it faster to explore less common configurations of chemical processes (Phimister and Seider, 2000a). Distillation, an energy intensive separation unit, has seen significant research in the area of process intensification in recent years. The intensified distillation technologies explored in this work are semicontinuous distillation, semicontinuous without middle vessel distillation and diving wall distillation.

Conventionally, distillation columns are used in batch and continuous operation, with each column separating a mixture into two different chemical streams. Semicontinuous distillation, on the other hand, uses a single column to separate any number of components, replacing the deleted columns with simple tanks. This type of process was first described by Phimister and Seider in 2000, demonstrating a ternary separation (Phimister and Seider, 2000b). Wijesekera and Adams demonstrated distillation processes that purify four or five components with one column and two or three middle vessel tanks (Wijesekera and Adams, 2015a). In the five-component configuration, the most and least volatile components are drawn as the distillate and bottoms streams of the column, while the three middle components concentrate in three middle vessels. This study used the results of the quintenary separation to generalize semicontinuous distillation to separate any number of components using one column and two less middle vessel tanks than components (Wijesekera and Adams, 2015b). As a result, there are endless applications for semicontinuous distillation.

The major advantage to operating a distillation column in a semicontinuous manner is the economic benefit. The capital investment required is greatly reduced compared to continuous distillation (Phimister and Seider, 2000a) and the operating costs are significantly lower than batch distillation. As a result, semicontinuous distillation is cheaper than both batch and continuous distillation for intermediate production rates (Adams and Seider, 2006).

Due to its economical and compact advantages, semicontinuous distillation is a great candidate to use as a separation unit used in the production of DME at petroleum well sites. Pascall and Adams studied semicontinuous distillation for the production of DME and were able to perform a ternary separation with the DME reaction by-products. In two different simulations, they were able to separate DME, methanol and water into three high purity streams (Pascall and Adams, 2013) and CO_2, DME, methanol and water into high purity CO_2 and DME while combining the methanol and water at the bottom of the column (Pascall and Adams, 2014). To date, the separation of CO_2, DME, methanol and water into four high purity streams has not been demonstrated with semicontinuous distillation in the open literature.

Semicontinuous distillation without a middle vessel (SwoMV) was developed to increase the throughput of the process and decrease the overall cost of traditional semicontinuous distillation. There are a few defining differences between the SwoMV and conventional semicontinuous distillation processes. The column is fed with fresh feed continuously in the SwoMV configuration (although at variable flow rates), and the destination of the side stream changes throughout each cycle. During the non-producing mode, the side draw is recycled and mixed with the feed stream to enter the column again. The purity of the side draw increases over the period of this mode. Once the purity of the intermediate component in the side draw meets an upper bound, the side draw is diverted from being recycled and is collected as product. During this mode, the purity of the side draw decreases until it meets the lower bound. At this point in time, the product stops being collected and the side draw returns to being recycled. The end result of the SwoMV configuration is a column that purifies the lightest and heaviest components at a variable continuous flow rates, and the intermediate component intermittently (Meidanshahi and Adams, 2015). The SwoMV configuration has been demonstrated for the purification of a benzene, toluene and *o*-xylene mixture (Meidanshahi and Adams, 2015), however no one has used it to separate DME from its reaction by-products or any four-component mixtures.

The dividing wall column (DWC) is another process intensification separation technology that operates more economically and energy favourably than continuous distillation systems. The DWC is run continuously to separate a three-component mixture in a single shell with a sheet partitioning the middle section of trays. The intermediate component accumulates on the right side of the wall and is directly withdrawn in a side draw stream. The most and least volatile components, are withdrawn as the distillate and bottoms streams. Since there is only one column and two heat exchangers to separate three components, this configuration not only has a lower capital cost, but also is more energetically favourable than continuous distillation (Yildirim et al., 2011). For certain situations, continuous DWC are cheaper than conventional continuous distillation (Yildirim et al., 2011).

The use of a dividing wall column for the purification of dimethyl ether has been studied and found to be more economical than the conventional DME separation route. Kiss and Ignat modelled the production of ultra-high purity DME, methanol and water using only one column by using a dividing wall column and by considering several different configurations (Kiss and Ignat, 2013). Kiss and Suskwalak combined reactive distillation with a divided wall column to dehydrate methanol to produce DME, methanol and water (Kiss and Suszwalak, 2012). Minh et al. separated the four one-step reaction by-products using only two dividing wall columns with significant energy savings compared to continuous distillation (Minh et al., 2012). Even though recent process intensification studies have made large advances in the efficiency of DME production, purifying DME from its one-step reaction by-products in a single column (a four species mixture) has not been shown yet.

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