AspenHysys Simulation of Methanol to Dimethylether (DME)

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ABSTRACT

Dimethyl ether can be used as a propellant, also can be used in diesel engines with the advantage of high efficiency, a high cetane number, and low exhaust emissions (no particulates, no Sulphur, and low NOx). Technical-quality DME is an alternative to liquefied petroleum gas (LPG). It has excellent combustion characteristics due to a low auto ignition temperature. Dimethyl ether has a cetane number of 55–60, DME can be used as a substitute for diesel fuel in a diesel engine.

This simulation study is able to predict and describe the compositions of the final production rate, and the distribution of the main components in the final product. This allows the estimation of economic factors, related to the operation of the catalytic reactor. For the present study, DME production process is simulated in Aspen Hysys V8.8 environment. a fluid package is selected along with the components which are to be in the input stream. In the process, NTRL was selected as the fluid package as it isable to handle selected pure components (methanol, water and dimethyl ether). The equilibrium reaction was selected to describe conversion of methanol to DME reaction.

Keywords

Aspen Hysys, Simulation, Methanol, Di-methyl ether

Introduction:

Dimethyl ether (DME) has received increasing interest as a potential substitutefor diesel and liquefied petroleum gas. The production of DME from syngas isexothermic in nature overall, and has a narrow operational window in fixed-bedreactors. Consequently, fluidized-bed reactors, which have high heat and masstransfer efficiencies, are major current areas of investigation for DME productionfrom syngas. In the present paper, the comprehensive reactor model proposed byMahecha-Botero et al. has been modified and employed to simulate DMEsynthesis in a fluidized-bed reactor. The modified model has been employedunder various operating conditions to maximize CO conversion (X_{CO}), DMEproductivity and DME selectivity with respect to methanol. [1]

DME also known asmethoxymethane, wood ether, dimethyl oxide or methyl ether,is the simplest ether. It is a colorless, slightly narcotic, nontoxic,highly flammable gas at ambient conditions, but can be handled as a liquid when lightly pressurized. The propertiesof DME are similar to those of Liquefied Petroleum Gas (LPG).

Currently, there are several licensors that offer technology for the production of DME based on a two-step process, including Haldor Topsøe, Lurgi, Mitsubishi Gas Chemical, Toyo Engineering Corporation and Uhde [**1**]

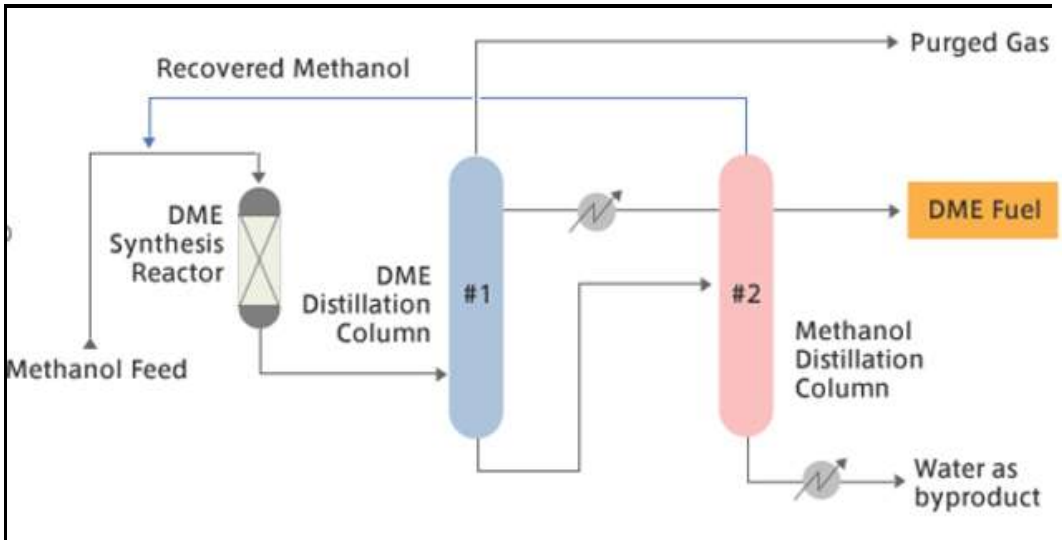

Fig (1): DME synthesis process (methanol dehydration)[6]

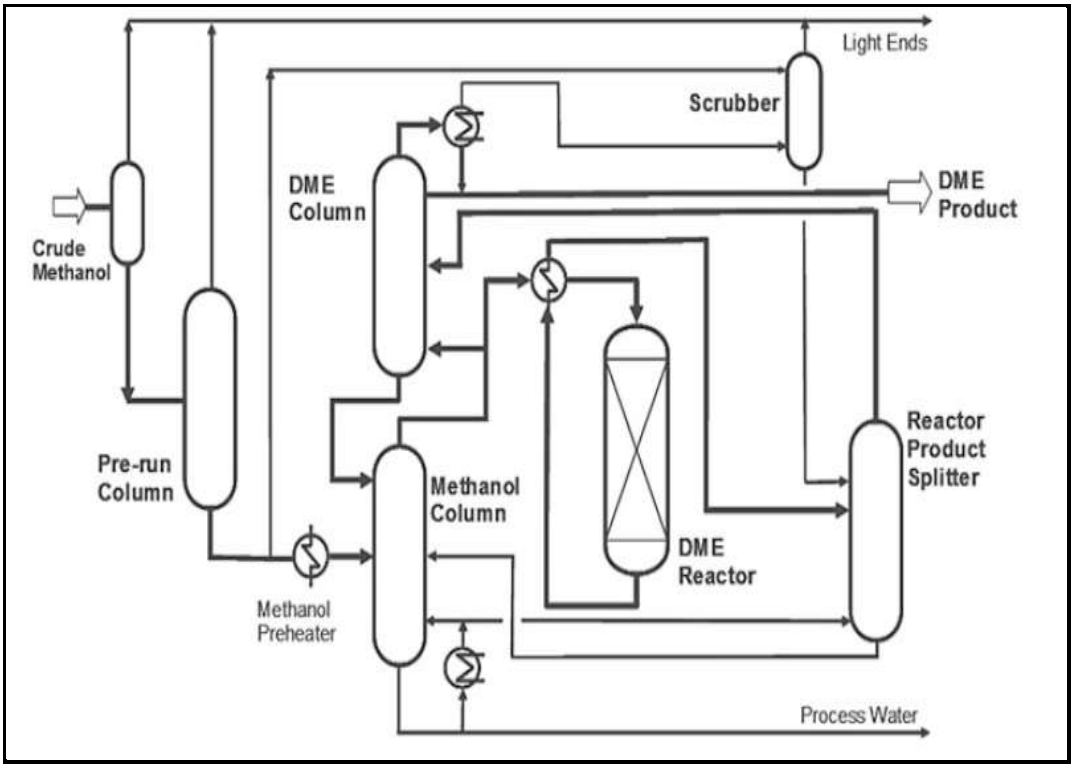

Fig (2): Dehydrating methanol over an acid catalyst (MT-DME). DME, dimethyl ether

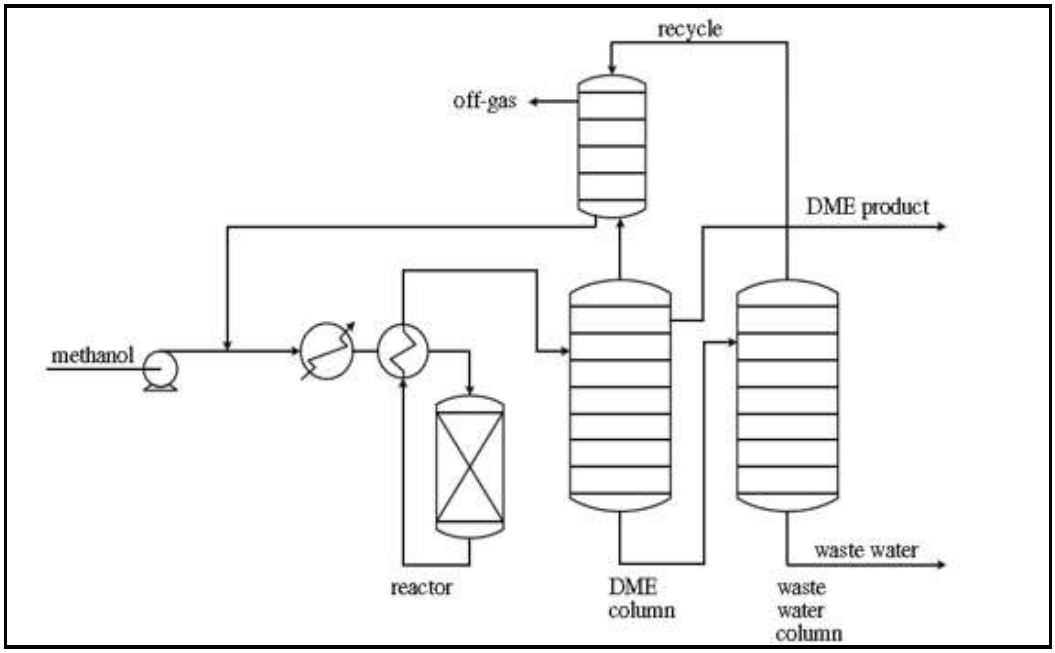

Fig. (3): Topsøe dimethyl ether (DME) Plan

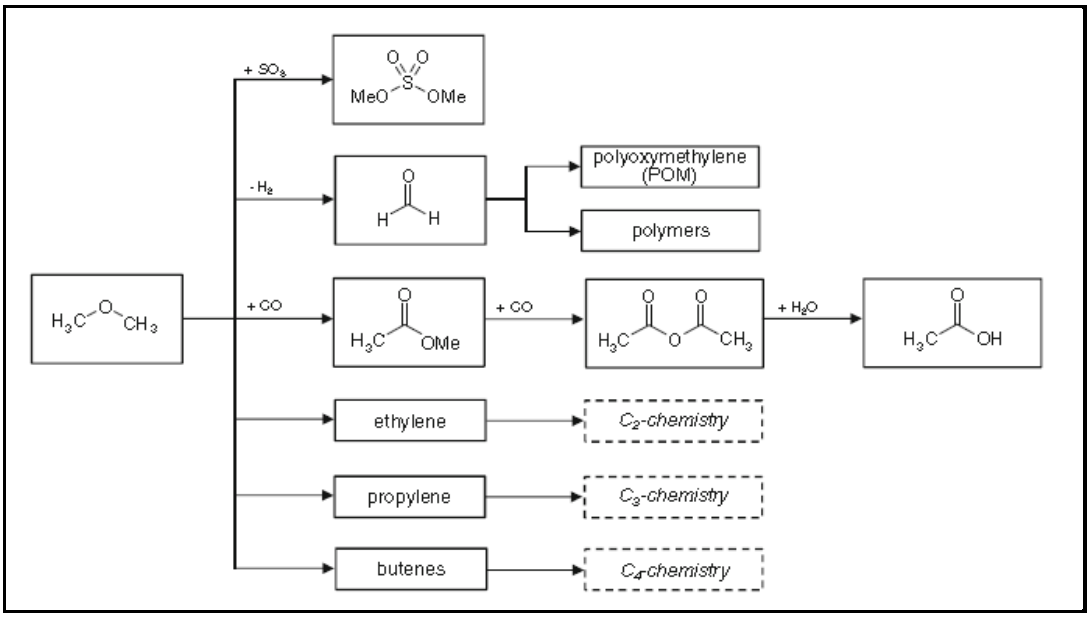

Fig (4): Dimethyl ether use in synthetic chemistry

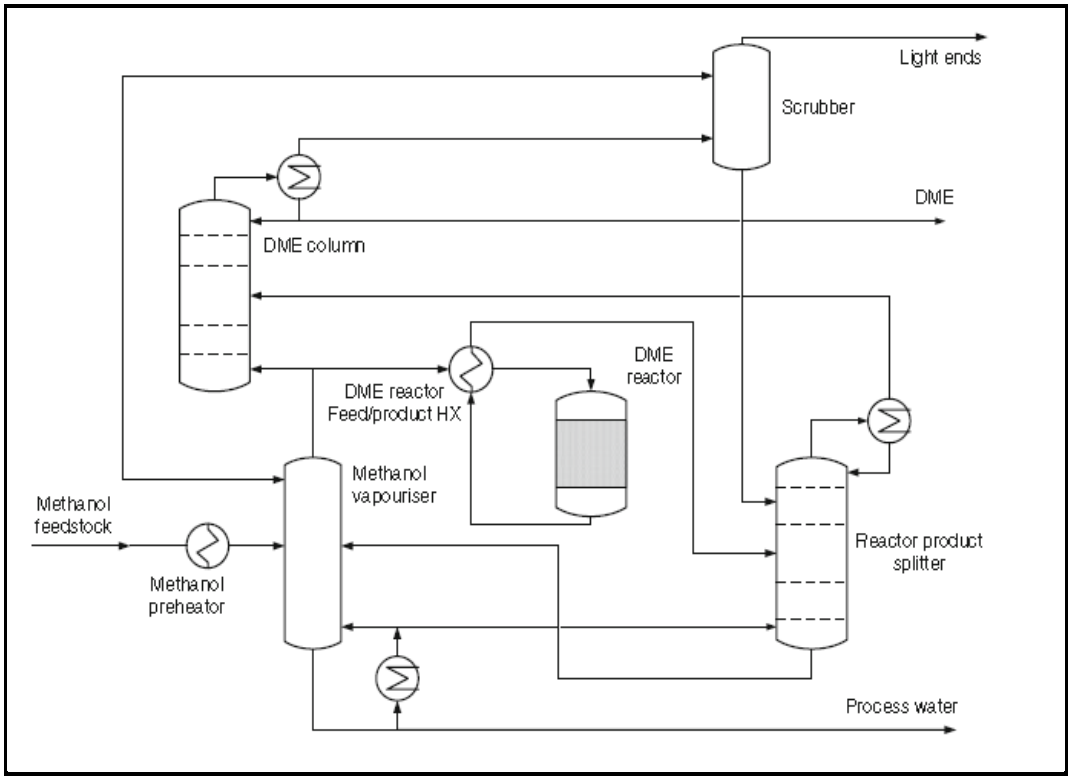

Fig (5): Lurgi's MegaDME process.

Experimental section

DME synthesis is a two-stage process. In the first step, methanol production is catalyzed over CuO/ZnO/Al_2O_3 at 50–100 bar and 270 _C. In a second step, CH_3OH is dehydrated in the presence of a Brønstedt or Lewis acidic catalyst, such as Al_2O_3, ZSM-5

The reaction of DME synthesis is mainly dehydration of methanol that is exothermic and reversible. In the current work, the rate expression has been selected from [3]

Methanol dehydration reaction: $2CH_3OH \Leftrightarrow CH_3OCH_3 + H_2O$ ΔH= –21,225KJ/mol.

Reactionkinetic

The reaction taking place is mildly exothermic with a standard heat of reaction of – 21,225KJ/mol

The equilibrium constant for this reaction at three different temperatures is givenbelow:

T (K)	K_p
200 C	34.1
300 C	12.4
400 C	6.21

Table (1): Reaction kinetic

The equilibrium conversions for pure methanol feed over the 200C-to-400C range are all greater than 83%. By limiting conversions to 80%, the reaction will not be equilibrium limited.

Process Simulator

Process simulator is defined as an engineering tool which performs automated calculations, mass &energy balances, physical property estimations, design / rating calculations, costing, process optimization, accurate description of physical properties of pure components and complex mixture, models for a large variety of reactors and unit operations, numerical techniques for solving large systems of algebraic and differential equations. [7]

In this work Aspen HysysV8.8 used to simulate production of DME.

Process Description:

Fresh methanol, (S1)vaporized priorto being sent to a fixed bed reactor, operating between 250C and 400°C. The single pass conversion in the reactor must be limited to 80% due to equipment constraints. The reactor effluent, (S9), is then cooled prior to being sent to the first of two distillation columns.

DME product is taken overhead from the first column. The second column separates water from the unreacted methanol. The methanol is recycled back to the front end of the process, while the water is sent to waste treatment to remove trace amounts of organic compounds.

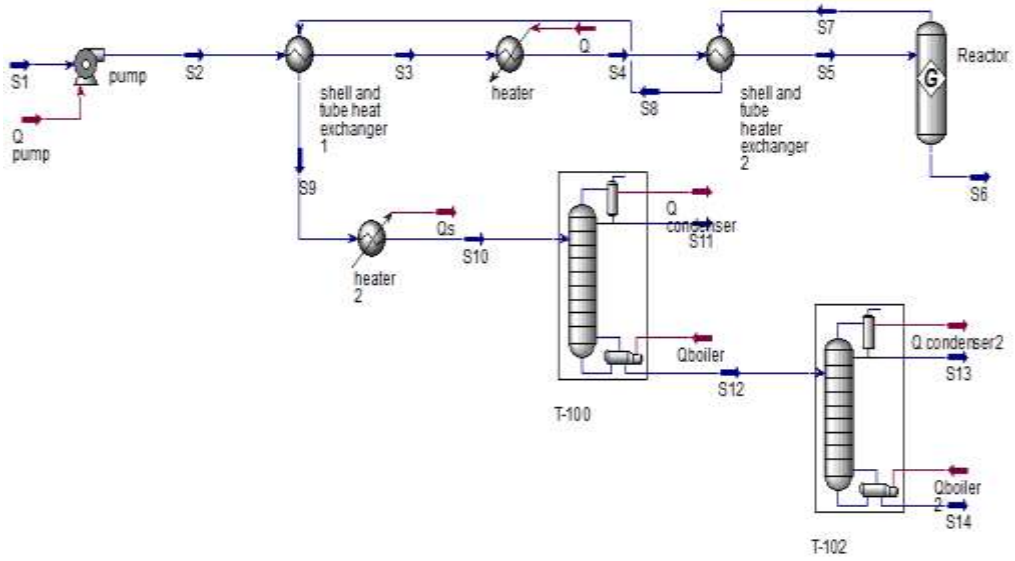

Fig (6): simulation of methanol to dimethyl ether by ASPEN HYSYS

Results and discussions

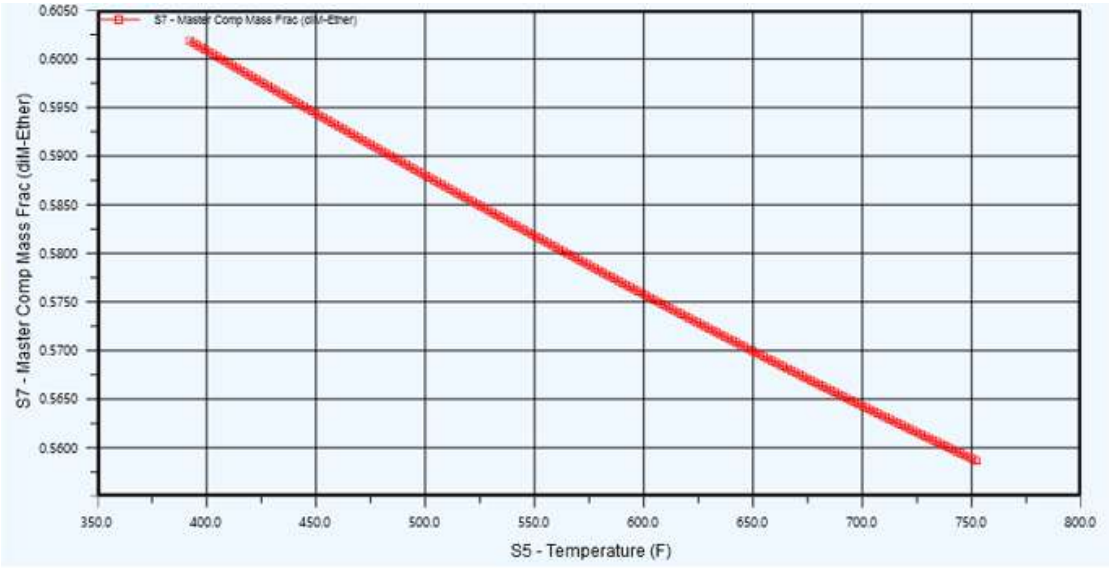

Fig (7): Temperature Vs Mass fraction of DME

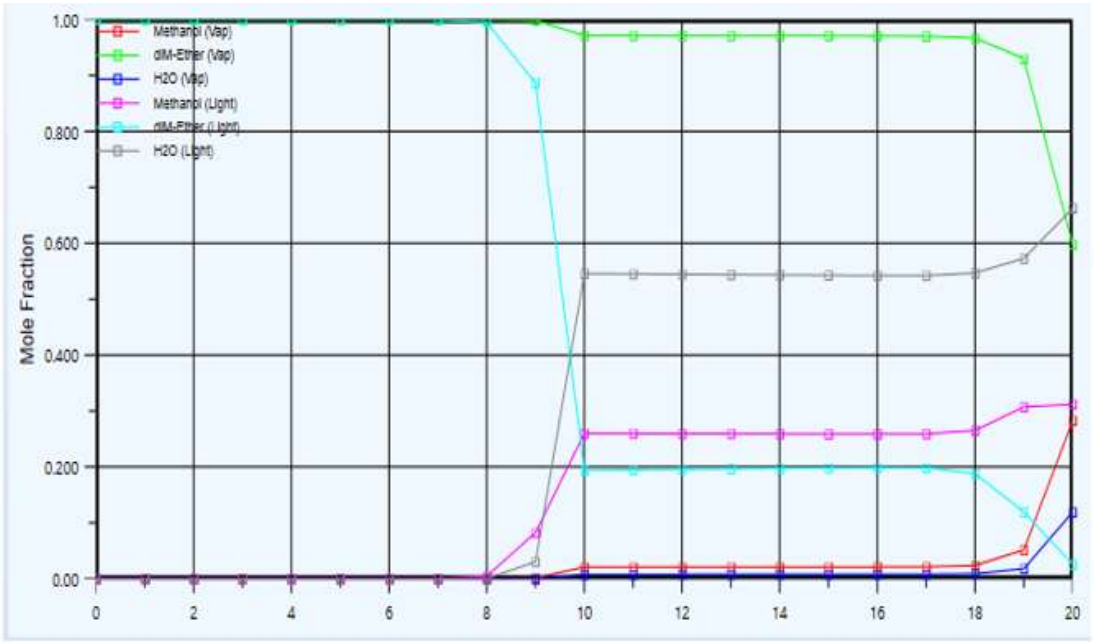

Fig (8):Composition Vs tray position from top

Conclusions

Simulation of a DME plant which is capable of producing DMEwith high purity (10,000 tonnes per annum) from methanol is done using ASPEN HYSYS V8.8 process simulator. NRTL is chosen as the property method in the simulation and assuming that 80% of the methanol is converted into DME in the equilibrium reactor, the product stream from the reactor consists of 41.16 % DME, 42.16 % water and 16.68%unconverted methanol. After passing through Heat exchangers (to bring down the temperature to the desired range for separation), the output stream is feed into distillation columns. Here, the separation into DME and water-methanol takes place.DME is separated from the firstdistillation columnas top product and methanol,water as bottom product, which fed into seconddistillation column.

Design specifications are used to meet the required results. The reflux ratios and the distillate rates are manipulated as variable parameters and the high purity of DME is obtained by using two distillation columns with fourHeat exchangers.

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