University of Alberta

Development and Implementation a Methodology for the Production of Dimethyl Ether from Methanol by Catalytic Distillation

by

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Abstract

This study reports on the development of a coherent solution methodology for the production of Dimethyl Ether (DME) from methanol using catalytic distillation. The validation and confidence of the Aspen Plus simulation results is first tested by simulating a catalyst distillation process for removing acetic acid from industrial wastewater stream. The simulation results correlate qualitatively well with the experimental data obtained by Xu et al., (1999). Using the methodology thus developed, the catalytic distillation column for the production of DME is designed by incorporating the Langmuir-Hinshelwood kinetic model developed by Hosseininejad et al., (2012). It is shown that synthesis of high purity DME can be achieved using a single catalytic distillation column. Parametric studies are used to determine the optimum tower diameter, tower hardware configurations, catalyst location and amount per stage as well as operating limitations.

Comparison of conventional and catalytic distillation processes using Aspen plus simulations show that there is a significant potential saving of total energy requirement for heating and cooling as well as reduction of plant size and capital cost for catalytic distillation column.

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Chapter 1

Introduction

There is awareness at all levels of society of two challenges faced today; climate change induced by global warming, and the threat of the diminution of energy supplies. Both of these challenges are driving the search towards alternative fuels and new sources for chemicals and liquid fuels traditionally based on petroleum. It is known that the dependence on oil and natural gas fuels to meet the increase in demand is limited due to the small reserve/production ratio. Thus on the demand side, it is necessary to try to conserve energy, while on the supply side, it is necessary to reduce the dependence on oil in the short term and convert to renewable energy forms in the long term. Fossil fuels such as oil, natural gas, shale gas, oil sands and coal will continue to be the main energy sources according to the demand forecast. The primary fossil fuels – oil, natural gas, and coal are non-renewable resources and are unevenly distributed around the world. Worldwide population and economic growth parallels consumption of fossil fuels. As a result, there has been increased awareness of a variety of issues such as greenhouse gases, energy security, and dwindling supply. These concerns lead to research and development of new type fuels that are more efficiency and cleaner energy supply. Also, the globally recognized fact that the use of fossil fuels in industry and society contributes more and more to climate changes is now gradually changing society's perceptions and attitudes towards the use of fossil energy. This new outlook about energy has enhanced people's awareness level and made them more alert in raising concerns about degrading air quality and global warming by the greenhouse gases (carbon oxides, nitrogen oxides, volatile hydrocarbons and chlorofluorocarbons etc.). As these problems are drawing our awareness, many changes have taken place, and more are being planned in the way fossil fuels are used. Most of the measures being taken to alleviate the worsening environmental situation are targeted at development of clean alternative fuels and relevant high-efficiency burning systems. These include such

notable alternative fuels as: gas-to-liquid fuels (GTL diesel and kerosene oil); methanol; dimethyl ether (DME); liquefied petroleum gases (LPG); and hydrogen.

Different from the primary fossil fuels oil, natural gas, and coal that are being heavily used these days, Dimethyl ether (DME) has been getting more interest of being used as an alternative to liquefied petroleum gases (LPG) and diesel when used as fuel. When there has been increased awareness of a variety of issues such as greenhouse gases, DME is a sulfur-free, near-zero aromatics synthetic fuel. DME has several physical properties similar to those of LPG. The weight-based heating value is higher than that of methane. The octane number is between 55~60, and DME has also found to possess cleaner burning characteristics as compared to conventional petroleum-derived diesel. Moreover, DME is non-toxic and reacts quickly in the atmosphere to form CO_2 and water. For these reasons, DME has been foreseen as a possible clean alternative fuel of future for electricity generation, domestic heating and automotive power. Some of the key advantages of DME for fuel use: it burns completely soot-free; as it is sulfur-free it does not produce sulfur oxides during combustion; it contains low nitrogen oxides; and it is non-corrosive, non-toxic and non-carcinogenic. It has a half-life of one day and it decomposes to water and carbon dioxide within a short time. Several of its physical properties are closely resembled with those of liquefied petroleum gas (LPG), a mixture of propane and butane(s), which impart DME the essential qualities of a clean burning domestic fuel. In addition, fuel-grade DME (a blend of DME, methanol and water with a small amount of an oxygenated additive) is said to be an excellent, and a superior, substitute for conventional petroleum-derived diesel fuel. DME, when compared with the combustion of conventional diesel, more cleanly and producing less carbon monoxide, nitrogen oxides (NO_X) and particulate matter. Being a sulfur-free fuel, another advantage of DME is that there are no sulfur compounds in the combustion products; in addition, formaldehyde, which is a regular constituent in the exhaust gases from the conventional diesel, is not formed in the case of DME.

Last but not the least, DME, as an oxygenated compound, is a potential replacement for methyl tertiary butyl ether.

Dimethyl ether is regarded as an alternative (clean) fuel derived from a non-petroleum source. Like methanol or middle-distillates (kerosene and diesel), DME can be produced from synthesis gas (a mixture of hydrogen and carbon monoxide gases produced from natural gas, coal, naphtha or heavy oils via reforming, coal gasification or partial oxidation technologies). Methanol itself is a source of DME, and the entire current commercial production of DME is based on it (via methanol dehydration technology). DME, in this way is envisaged as a potential competitor for methanol, LNG and GTL fuels in the context of utilization of the remote (or stranded) natural gas or coal lying untapped due to economic and environmental constraints. DME is a kind of oxygenate compound, thus when blended with diesel or gasoline results in oxygen boost which leads to decrease in amount of carbon monoxide and hydrocarbons in the exhaust stream. Although alcohols have the same characteristic of having oxygen in the compound, ether is better choice because of their low vapor pressure behavior. DME can also be used as a raw material of many products, such as short olefins (ethylene and propylene), gasoline, hydrogen, acetic acid and dimethyl sulfate. It is easy for transporting DME to areas far from the oil and gas production place.

At the present time, almost all commercial DME is produced by dehydration of methanol using acidic porous materials such as zeolites, silica-alumina, alumina, Amberlyst 35, etc. as the catalyst. Solid catalysts are chosen because they can be easily separate from reaction mixtures. Methanol can be synthesized from syngas, which is usually produced from natural gas, coal or biomass sources. The methanol dehydration reaction can be presented globally as:

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \quad (1)$$

Presently, commercial DME processes use an acidic catalysts packed bed reactor to dehydrate methanol, followed by a distillation column to separate DME. Catalytic Distillate (CD) is an alternative process combining a reaction zone

packed with acidic catalyst for dehydrating methanol and multistage distillation to separate high purity DME in single column.

There are several important advantages of the CD process over the conventional process; the heat of reaction can be used in distillation, limitations imposed by thermodynamic equilibrium of the reaction are overcome by continuous removal of product from the reaction zone (Gates and Johanson, 1971), reduced downstream processing of separating and purifying DME. The CD process offers lower cost in operation, and better quality of product when compared with the conventional processes. Combining reaction and separation within one vessel also reduces the overall capital cost compared with use of separate vessel for each process.

The objective of this study is to develop and implement a methodology for the production of DME from methanol using Catalytic Distillation. Both the traditional and CD processes will be compared using Aspen Plus simulation software to provide a clear detail of the energy requirements of both processes. Also providing key design parameters of a CD process and further discussion of a detail column characteristic will be shown in the simulation.

Chapter 2

Development of Process Simulation Methodology

The main goal of this study is to use experimentally determined kinetic data and an appropriate thermodynamic model to simulate and optimize a full-scale process to produce dimethyl ether. To develop an accurate methodology for designing a reactive distillation column, it is best to compare simulation results to published experimental data from similar reactive distillation processes. However, in the case of DME production using reactive distillation, the published experimental data are very scarce in the open literature. Therefore, to validate the code, the simulation results will be compared to data from Xu et al., (1999).

Xu et al., (1999) used a catalytic distillation process to remove acetic acid from a chemical/petrochemical plant's wastewater stream. Acetic acid is produced as a by-product while manufacturing terephthalic acid, dimethyl terephthalate, acetic acid, esters involving the uses of acetic anhydride, cellulose acetate and acetat rayon in industrial chemical plants. The major challenge of recovering acetic acid from these streams involves the separation of the acid from relatively large amounts of water.

A novel process to purify the acetic acid uses catalytic distillation by introducing a methanol stream in to the column, letting acetic acid react with methanol to form methyl acetate while easily separating methyl acetate from water. This method lowers the energy consumption and also reduces corrosion problems caused by the acid compared to a conventional distillation process.

Acetic acid reacts with methanol to form methyl acetate and water as shown below:

$$CH_3OH+CH_3COOH\leftrightarrow CH_3COOCH_3+H_2O \qquad (2.1)$$

The kinetic model for this reaction was determined from experimental data, which used the solid-acid catalyst Amberlyst 15 to accelerate the reaction. The rate law was then determined using the Langmuir-Hinshelwood model for a heterogeneous

reaction in which it is assumed that the adsorption is weak for all components. The reaction can be expressed in a familiar power law model:

$$\frac{\mathrm{dC_{MeAc}}}{\mathrm{dt}} = \mathrm{k_2}(\mathrm{C_{MeOH}C_{HAc}} - \mathrm{C_{MeAc}\,C_{H_2O}/K}) \tag{2.2}$$

where C_j is the concentration of adsorbed component j and k_2 is a function of temperature and catalyst loading. It can be calculated by plotting the reaction rate over the concentration and expressed as follows:

$$\mathrm{k_2} = k_0 W exp(-\frac{E}{RT}) \tag{2.3}$$

where W is the catalyst loading, k_0 is pre-exponential constant (1.76×10^6) and E is the activation energy which is 58.5 kJ/mol. Also, from Equation (2.2), K is the apparent equilibrium constant of the reaction and is found from:

$$\mathrm{K} = \frac{\mathrm{C_{MeAc,e}C_{H_2O,e}}}{\mathrm{C_{MeOH,e}C_{HAc,e}}} \tag{2.4}$$

The Equilibrium constant K is reported by Agreda et al. (1990) to be 5.2 and reasonably independent of temperature. This information can be used to build a kinetic model to simulate the reaction in Equation (2.1) using Amberlst 15 as the catalyst. The final kinetic equation is given by:

$$\frac{d\mathrm{C_{MeAc}}}{dt} = k_0 W exp\left(-\frac{E}{RT}\right)\left(C_{MeOH}C_{HAc} - C_{MeAc}\,C_{H_2O}/K\right) \tag{2.5}$$

Figure 2.1 shows the process diagram of the process. Low concentration acetic acid is fed from the stage 2 of the column and pure methanol is fed at stage 6. Catalyst beds are installed in the column between each tray. In total there are seven separation trays which are conventional dualflow trays; five reaction zones which are a catalyst unit composed of a catalyst basket filled with a solid acid catalyst Amberlyst 15 and placed between two dualflow trays in the column. Notice that there is not a reaction zone between tray 1 and 2 in the column.

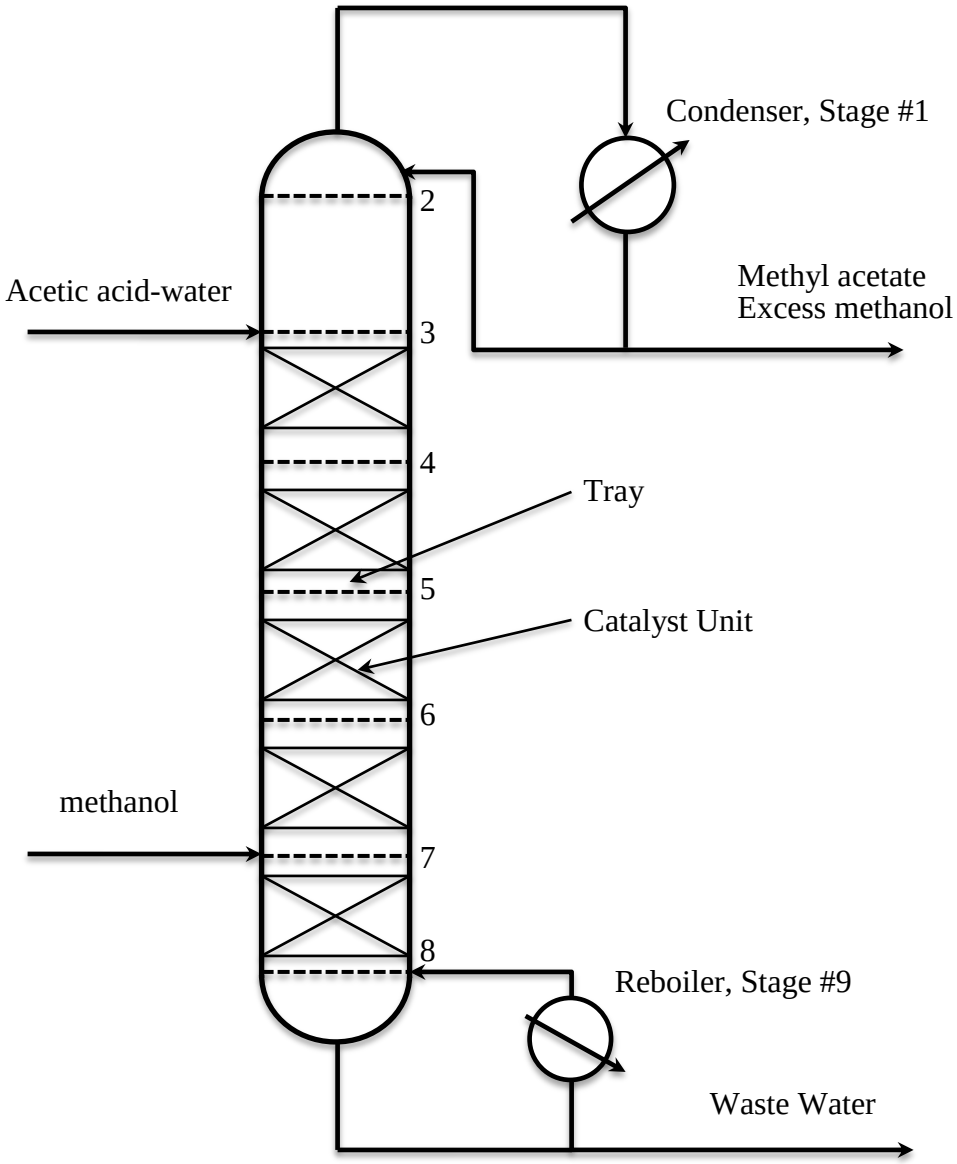

Fig 2.1 Column detail for removal of acetic acid by catalytic distillation.

The experiments were done in a column with a diameter of 100 mm and a height of 1.5m. For the experimental study, Xu et al., varied several characteristics to generate 33 different runs for which data was recorded. They varied the feed composition and flow rate, reflux ratio and column pressure. The experiments are designed using the following specification ranges: the acetic acid feed contains 2 to 10 wt% of acetic acid in water at a rate of 100 to 300 g/min; the methanol (pure methanol) feed rate was varied from 5 to 50 g/min, the top product rate was controlled between 5 to 50 g/min; the bottom product rate was controlled between 100 to 300 g/min; and the reflux ratio was set from 5 to 25.

After collecting the experimental data, a comparison of both simulation result and actual data are done by building the simulation using the kinetic reaction given from Equation (2.5). Aspen Plus was used as the simulation package using the ideal gas and Henry's law for the vapor phase and NRTL (Non-Random Two Liquid model) model for the liquid phase and to calculate the liquid-vapor equilibrium by minimizing the Gibbs free energy. Each catalyst unit placed between two dualflow trays in the catalytic distillation column is modeled as a continuous stirred tank reactor (CSTR).

Only run #10 from Xu et al., (1999) is compared to simulation results. They provided a full input data and output Aspen file for only this run. Therefore, it is the only run in which it was possible to represent the simulation data accurately. Table 2.1 shows the input data for experimental run #10. For simulation this run, the liquid holdup on each catalyst unit is 0.027 m^3, which is used as the input amount of catalyst in the reaction kinetic law template. Component Murphree tray efficiencies are set for the separation stages as stated in the Aspen input file from Xu. The reflux, distillate rate, bottom product rate and column pressure are all set to the values shown in Table 2.1. The detailed input and output files from Aspen are also listed in Appendix A.

Table2.1 Detail input settings of experimental run #10

Run#	10
MeOH Feed (g/min)	30
Acetic acid Feed stream (g/min)	140
Acetic acid in Feed (Wt %)	5
Catalyst Unit	3-7
Reflux Ratio (mole)	8.75
Pressure (kPa)	93.5
Top product rate (g/min)	17.54
Bottom product rate (g/min)	153.5

Figure 2.2 shows a comparison between the simulation results obtained using ASPEN Plus and experimentally measured concentration profile of each component as a function of tray location. It should be noted that in the figure the tray number is counted from the condenser to the reboiler, (i.e, the compositions measured from the condenser are shown in the figure as the compositions on tray 1 and those form the reboiler as tray 9). Experimental data are read from a log scale figure in Xu et al., (1990) study.

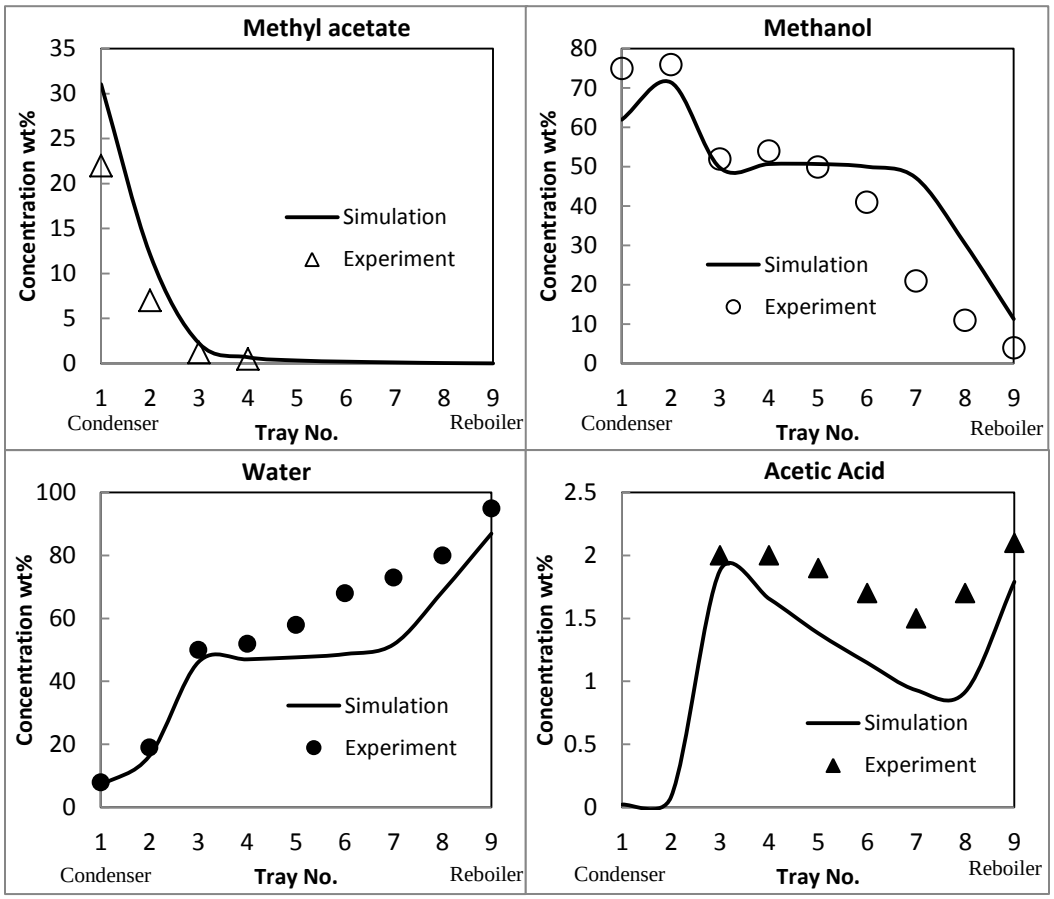

Fig 2.2 Comparison of the simulation results and the measured concentrations of each component as a function of stage location for Run #10.

In Fig 2.2, the component concentration on each tray inside the column shows the simulation results correlate qualitatively well with the experimental data trends. The methyl acetate concentration starts high in the top of the column but quickly reduces to zero after the reaction stages start between trays 2 and 3. At the top of the column the measured composition is 9% lower than the simulated composition. To balance this difference, the simulated methanol composition at the top of the column is 13% lower than the measured composition. These differences in compositions at the top of the column could be due to assumptions made while simulating the process. The simulated column does not consider heat loss, and subcooling of the refluxed liquid at the top of the column. At the bottom of the column the simulated results predict 7 % more methanol with 8 % less water. These differences could be due to the reasons mentioned above, as well as the estimated Murphree stage efficiencies used in the simulation. The amount of acetic acid in the bottom of the column, and the similar concentration profile for acetic acid shows that the reaction zones are predicting the behavior properly. Overall, the simulation and experimental results both show a 60 % conversion of acetic acid. The methanol and water concentration profiles seem a bit stagnant in the simulation between stages 3 and 7. It was expected that both composition profiles stay flat only between stages 3 and 5, then start to change. These differences could be due to the estimated stage efficiencies used in the simulation.

Fig 2.3 shows the component compositions of the liquid phase profiles within the catalytic distillation column using different estimated Murphree stage efficiencies. It can be seen that the change in Murphree stage efficiencies for every component on each stage affects the simulation result. Therefore, the measurement for Murphree stage efficiencies from experiment is necessary. The experimental data then can be used to validate simulation results and modify input models.

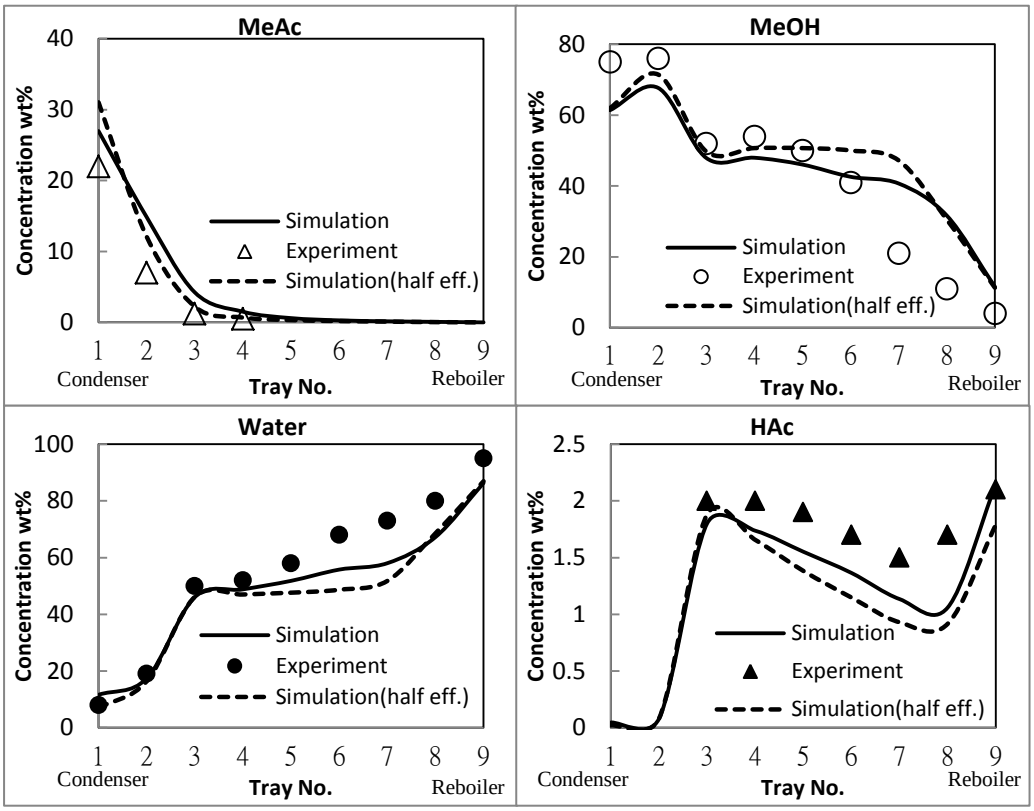

Fig 2.3 Changes of Murphree efficiencies affecting simulation results.

From these results, the code used to predict the behavior in a reactive distillation column using Aspen Plus is validated. From the concentration profiles of all components in the column it can be seen that there is both reaction and separation occurring, similar to what is seen experimentally. With a valid kinetic reaction model and know stage efficiencies, it is therefore reliable to use Aspen Plus simulation package for the purpose of predesigning a catalytic distillation process.

Chapter 3

Implementation of the Methodology for the Production of DME from Methanol

In the previous chapter, the methodology of designing of a catalytic distillation column was confirmed with experimental data obtained by Xu et al., (1999) for removal of acetic acid from wastewater. In this chapter, we will further develop a coherent methodology for the production of DME via the catalytic distillation process by incorporating the two kinetic models aforementioned above.

To design and simulate the catalytic distillation column process, the reaction kinetics information is needed. Many investigators agree that the dehydration of methanol to DME on solid-acid catalyst, the mechanism follows Langmuir–Hinshelwood (Gates and Johanson 1971) or Eley-Rideal kinetics model (Kiviranta-Paakkonen et al., 1998), with water and DME both acting as reaction inhibitors. The main difference of both reaction models is that Langmuir–Hinshelwood model assumes two methanol molecules occupy two adjacent acid sites. On the other hand, the Eley-Rideal model claimed that only one methanol molecule adsorbs on the acid site, which reacts with a second molecule from the liquid bulk phase.

Solid-acid catalysts are mostly used in catalytic dehydration of methanol to DME. Silica-Alumina, γ-Alumina, and different kinds of zeolites, namely, Mordenite, ZSM-5 and Y show good methanol conversion and selectivity to DME at high temperatures and pressure. However, ion exchange resins are preferred over acidic zeolites as catalyst for the methanol to DME process because they required relatively low operating temperatures and having high selectivity to DME (Spivey 1991). The best choice catalyst should be combination of strongest acid strength and highest number of active sites and resistance to water inhibition and side product formation.

Weizhu et al., (2004) investigated liquid catalytic dehydration of methanol over an ion exchange resin (Amberlyst 35) using batch slurry reactor in the

temperature range of 70 to 130 ℃ and initial reaction pressure of 0.82 MPa. They described experimental data using an Eley-Rideal type kinetic expression, in which the rate-determining step is mainly depends on the surface reaction on the catalyst. They indicated that that adsorption of the more polar components (methanol and water) are much stronger than the adsorption of the less polar component such as ether (Linnekoski et al., 1997) and they have proposed the following the kinetic model

$$r_{DME} = \frac{k_S C_M{}^2}{\frac{K_w}{K_M} C_W + C_M} \tag{3.1}$$

where k_S is the surface reaction rate constant and they defined as :

$$k_S = k_0 \exp(-E_a/RT) \tag{3.2}$$

The reaction constant, k_S, was found by gathering the initial reaction rate in the absence of water. The experimental data gave k_0 value to be 4.72 m^3/kg cat.s and active energy E_a of 51.7 kJ/mol. They have also investigated the effect of water presence on the initial reaction rate. Water and methanol compete for adsorption at the catalytic active sites on the surface of acid catalysts. They have shown that increasing water concentration will lower the reaction rate in the mixture. From their experimental data, the have found the relationship of the ratio of adsorption equilibrium constant of water to methanol as:

$$\frac{K_w}{K_M} = \exp(-25.75 + \frac{11138}{T}) \tag{3.3}$$

Hosseininejad et al., (2012) also studied kinetics of dehydration of methanol to DME over Amberlyst 35. The reaction was carried out using an autoclave batch reactor in the temperature range of 110 to 135 ℃ and initial reactor pressure of 0.9 MPa. They described their experimental data well using the Langmuir-Hsinshelwood kinetic expression, in which the surface reaction is the rate-determining step. In the absence of water, they proposed the following the reaction kinetic model:

$$r_{DME} = \frac{k_S C_M{}^2}{\left(\frac{K_W}{K_M} C_W + C_M\right)^2} \quad (3.4)$$

where, k_s is the surface reaction rate constant, k_s was determined by

$$k_S = k_0 \exp(-E_a/RT) \quad (3.5)$$

The experimental data gave k_0 value to be 6.12×10^7 mol/kg cat. s and active energy E_a of 98 kJ/mol for the temperature range of 110-135 ℃. They also examined the effect of water presence on the initial reaction rate. From experimental data, they proposed the temperature dependence of the ratio of adsorption equilibrium constants of water and methanol with following equation

$$\frac{K_W}{K_M} = \exp(-6.46 + \frac{2964}{T}) \quad (3.6)$$

It is clear from the literature that the best choice of catalyst is Amberlest 35 because catalytic distillation of DME takes place at relatively low pressure (0.8 to 1.2 MPa) and temperature in the range of 50-180 °C.

Weizhu et al., (2004) and Hosseininejad et al., (2012) kinetic models were developed using the same catalyst type (Amberlyst 35). Comparison of these kinetic models will allows us to determine which kinetic model is more suitable for future optimization design for the DME production using catalytic distillation process.

In this study, RadFrac, rigorous equilibrium stage model build in the Aspen Plus simulation package was used to simulate the catalytic reactive distillation process for methanol dehydration to DME. In these simulations, the vapor-liquid equilibrium data was obtained using NRTL (Non-Random Two Liquid) equilibrium stage model and it was assumed that there was no pressure drop across the column, which allows us to specify the operating pressure via the condenser pressure. It is important to indicate that the distillation tower pressure was set 0.9 MPa to ensure that the reaction will take place in the liquid phase. Both kinetic models were used with user kinetics subroutine for the program

REAC-DIST to calculate the liquid phase generation rate for each component at each stage in the reaction zone.

Figure 3.1 shows the flow diagram of simulation CD process. A series of simulation were performed using kinetics models developed by Weizhu et al., (2004) and Hosseininejad et al., (2012). For both kinetics models, the total number of total stages was 30 and the reaction zone was kept in between 8 and 20 stages and striping section was in between 21 and 30 stages. In the reaction zone, catalyst loading was 9.23 kg/stage. The pure methanol was feed into the column just above the reaction zone (i.e stage 8) and high purity DME product was collected from the condenser while water was collected at the bottom stream from the reboiler. For all simulations, the feed rate and reflux ratio (V/L) were kept constant at 2.5 mol/s and 9, respectively.

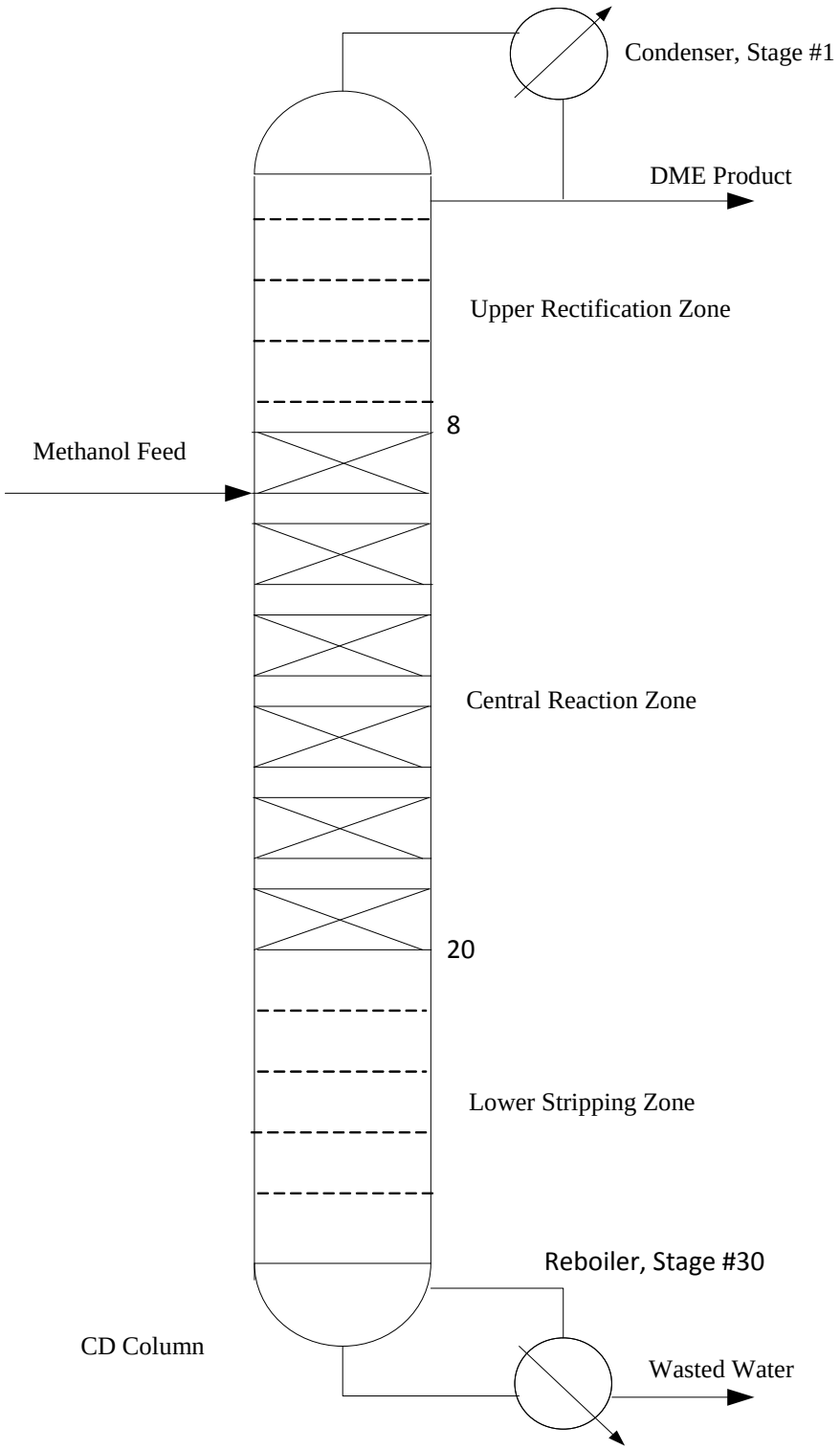

Fig 3.1 Catalytic Distillation process simulation flow diagram.

Figures 3.2 and 3.3 show the component compositions of the liquid phase profiles within the catalytic distillation column using Eley-Rideal and Langmuir-Hinshelwood models, respectively. Both figures show that DME is more volatile than either water or methanol and was collected as the overhead product while water, which is the least volatile component, was collected at the bottom of the column. Methanol was retained inside the column due to boiling point and converted to DME and water.

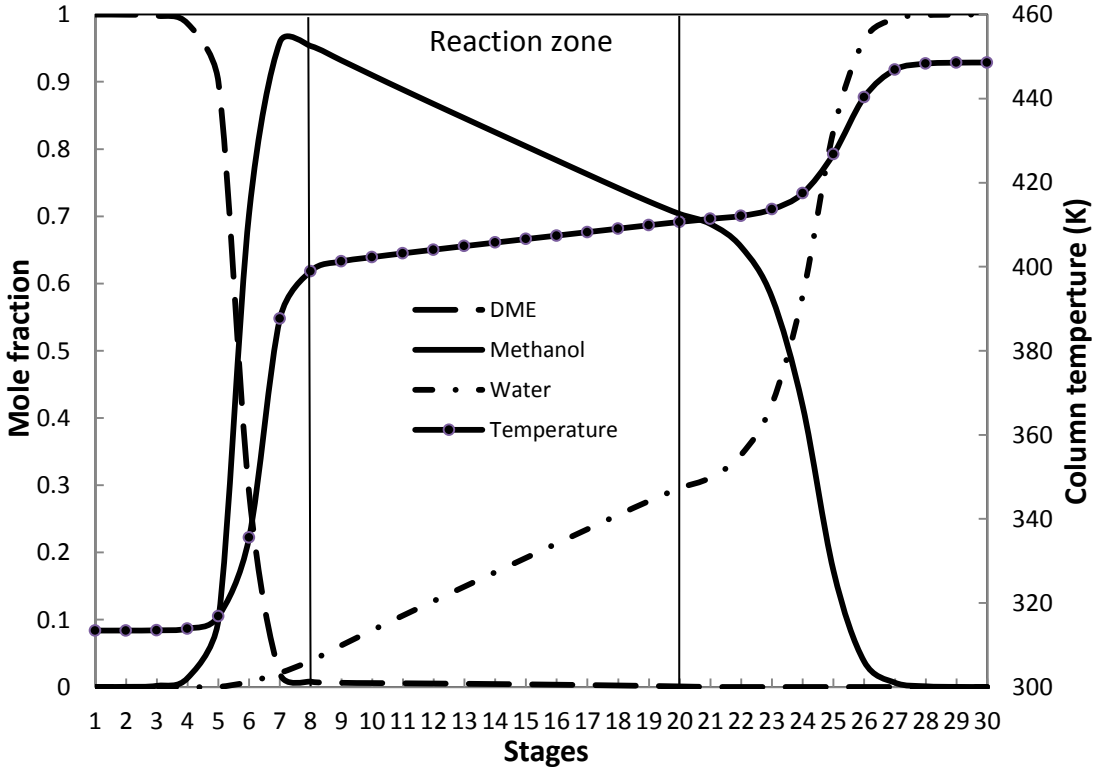

Fig 3.2 Liquid-phase composition and corresponding temperature profiles obtained using Eley-Rideal reaction kinetic model.

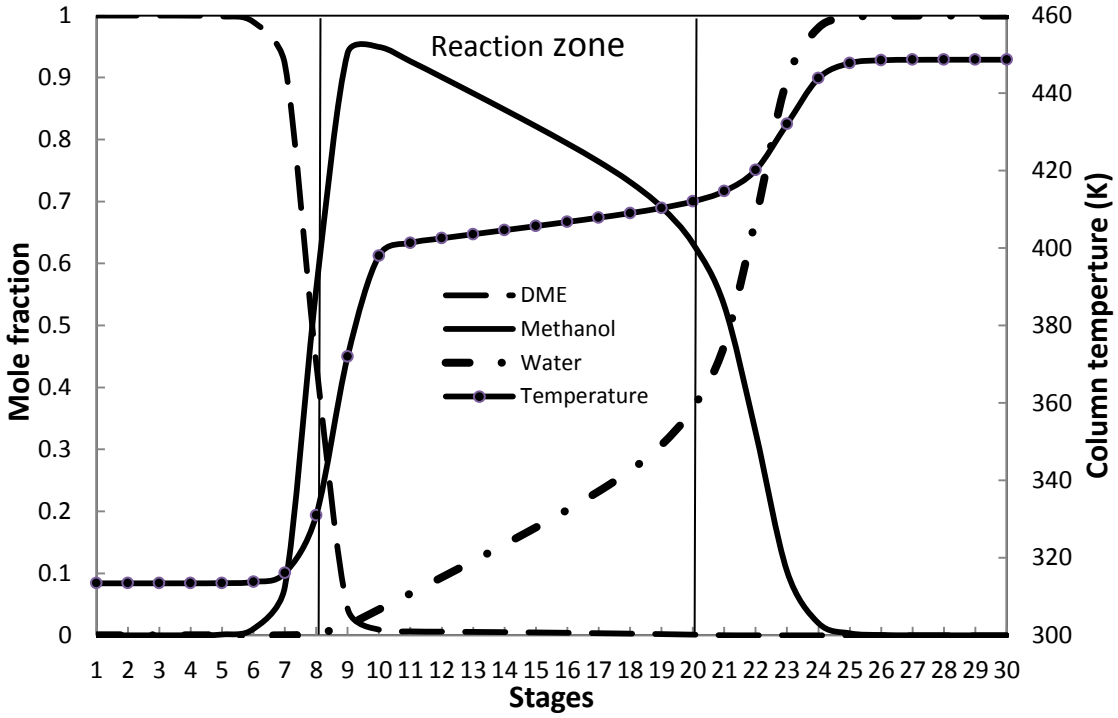

Fig 3.3 Liquid composition and corresponding temperature profiles obtained using Langmuir-Hinshelwood reaction kinetic model.

Both figures also show that the two kinetic models show similar performance, reaching the goal of 99.99 mol% purity of DME. The Langmuir-Hsinshelwood kinetic model developed by Hosseininejad et al., (2012) shows faster reaction in the reaction zone which would lead to fewer stages for the process as shown in Figure 3.3.

To summarize, a proper methodology and kinetic model are essential for the design of industrial columns, such as for the optimum design of the internals with the optimum design of the column internals with optimum combination of catalyst bed and separation trays for reaction and separation.

Chapter 4

Configuration and Parametric Studies

In this chapter, parametric studies were conducted using the kinetic model of Hosseininejad et al., (2012) and the equilibrium model to study design and operating strategies of the catalytic distillation process. A number of simulations were performed to determine which parameters affect the column performance. Based on the starting specs given in Table 4.1, the following parameters were investigated: the total number of theoretical stages, the location of the feed stage for liquid methanol, reflux ratio, catalyst loading per stage in the reaction zone, the number of stages for the reaction zone and positioning of the reaction zone. These parameters were varied independently. The main objective of all simulations is to achieve 99.99 mol% DME purity in the top product stream.

Table 4.1 Input parameters for simulation of catalytic distillation of methanol to DME

Feed Stream		CD Column	
Temperature	298 K	Total stages	30
Pressure	0.9MPa	Rectification stages	1-7
Flow rate	2.5 mol/s	Reaction stages	8-20
Feed composition	Pure Methanol	Stripping stages	21-30
		Feed stage	8
		Catalyst loading	9.23 kg/stage
		Column pressure	0.9 MPa
		Reflux ratio	9
		Distillate to Feed Ratio	0.5
		Column Diameter	0.33 m

Total number of equilibrium stage

The optimum number of equilibrium was determined by varying the total number of stages between 15 and 40, and the size of the reaction zone was always kept constant at total of 13 stages for each set of simulation. Figure 4.1 shows the DME concentrations in both liquid and vapor phases as a function of total number of stages. It can be seen that the purity of DME improved as the total numbers of stages were increased up to 25 stages. However, there was no significant improvement over 25 stages. Furthermore, all above simulations also shown that water concentration in the bottom stream from the reboiler reaches 99.99 mol% when total number of stages increased to 25. The purity of the DME and water products was each increased to nearly 100 mol% when a total number stages chosen to be 30 and having a 13-stage reaction zone.

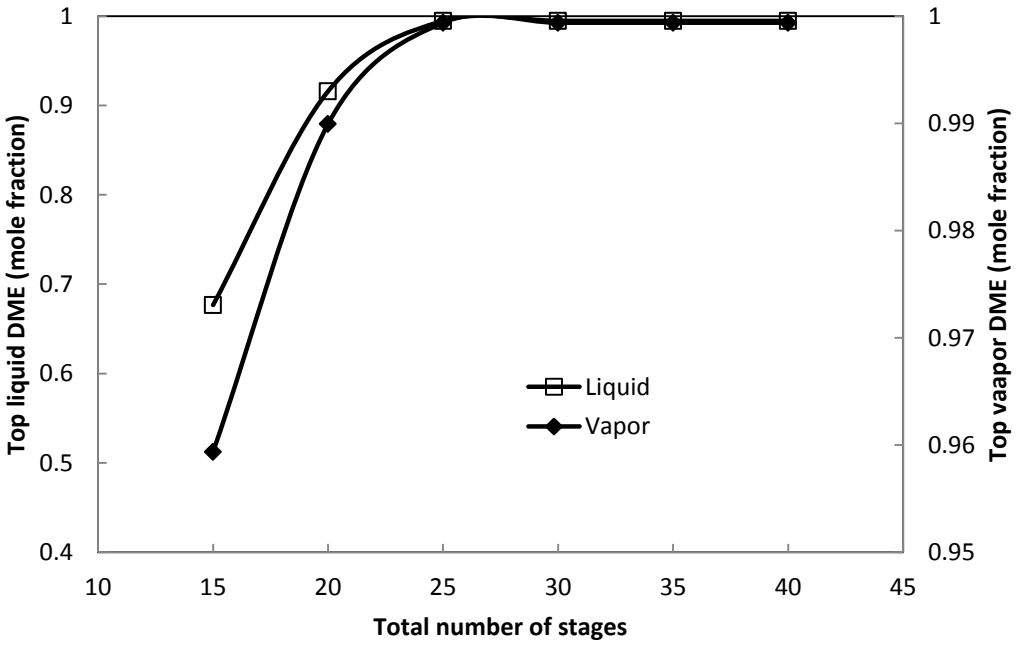

Fig 4.1 Effect of total number of stages on DME concentration.

Feed stage location

Figure 4.2 shows the effect of feed stage location on purity of DME in the top product stream. The optimum feed stage location was determined by varying that location between stage 6 to 24 while the reaction zone was kept between stages 8 to 20 of a total of 13 stages. It can be seen that the DME concentration in the vapor and liquid phases at the top of the column was maximized by feeding methanol just above the reaction zone, between stages 6 and 8. The results shows that feeding methanol at the start of the reaction zone produces higher concentration of DME in the condenser due to the reaction rate is the highest and product of water and DME are removed from the reaction right away can cause the converting rate of methanol to be maximized. Figure 4.2 also shows that when methanol feed is at the bottom of the reaction zone or even lower than the reaction zone it causes the conversion of methanol is reduced and lead to lower purity of the DME product. Therefore, the optimum position for methanol feed should be just above of the reaction zone.

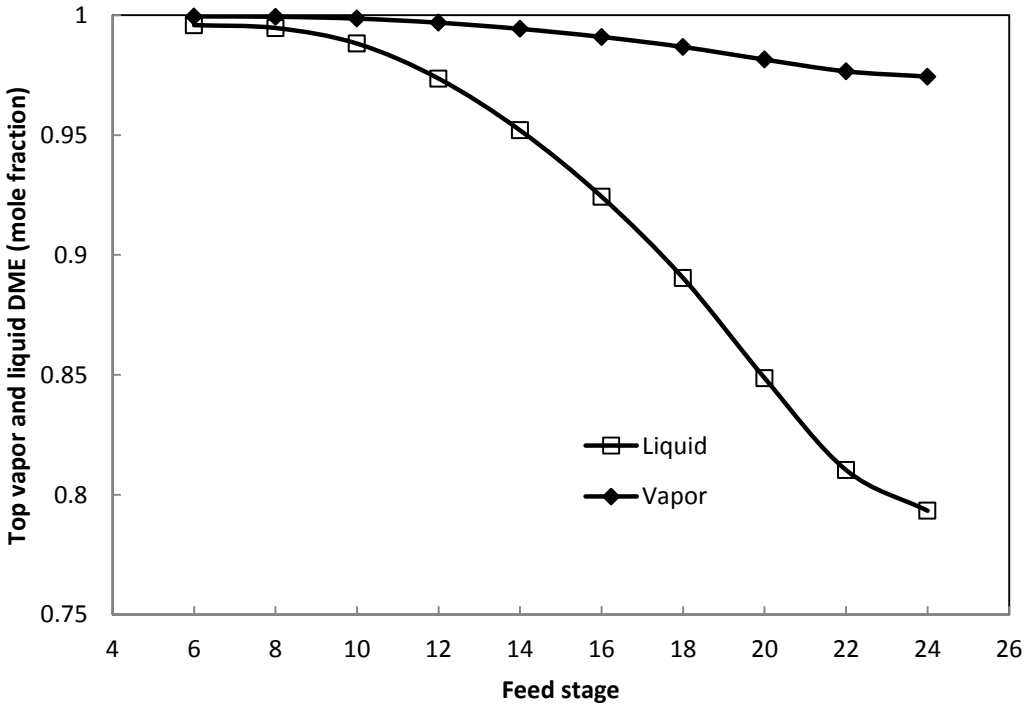

Fig 4.2 Effect of feed stage location on DME concentration.

Reflux ratio

Subawalla and Fair, (1999) have indicated that reflux ratio affects both reaction rate and separation performance in the CD column. At higher reflux ratio methanol recycle increases inside the reaction zone and this leads to increase the local methanol concentration and so increases the driving for the reaction. The simulation results shown in Figure 4.3 indicates that high purity of DME (100 % as top product) can be obtained at reflux ratio 9 for catalyst loading of 9.23 kg per stage. Furthermore, increasing reflux ratio will increase the residence of methanol in the reaction zone and hence could reduce the required catalyst loading per stage, which will be further discussed in the next section. On the other hand higher reflux ratio will result higher operation cost for both condenser and reboiler duties and also the column diameter will need to be increased to accommodate higher flow traffic inside the column.

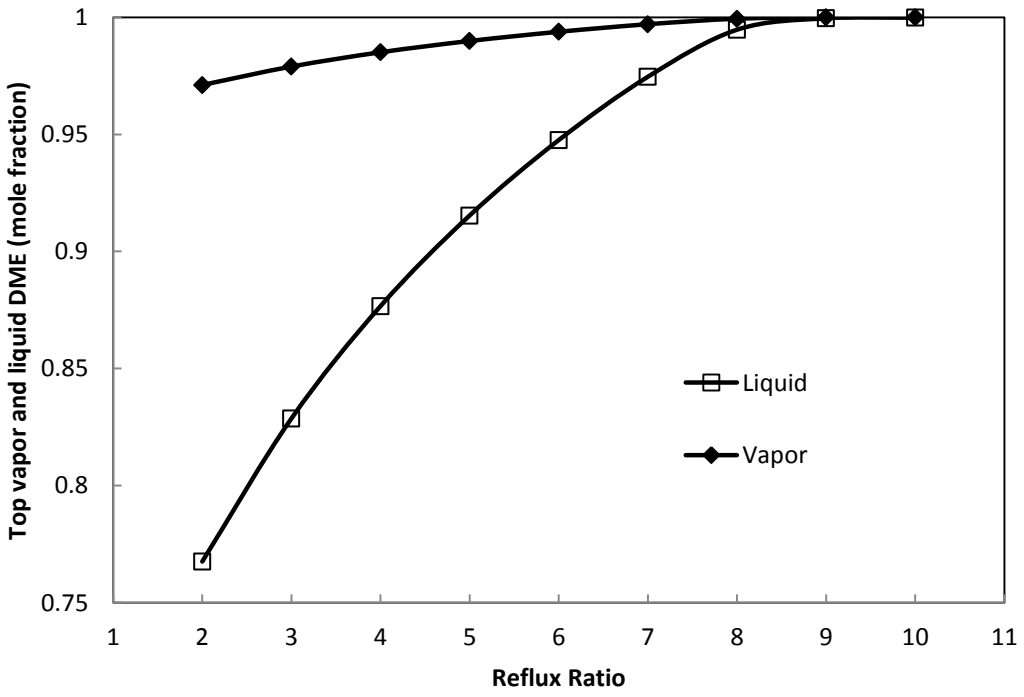

Fig 4.3 Effect of C on purity of DME in the top product.

Catalyst Loading

Amount of catalyst loading on each stage in the reaction zone is the main key parameter, which will affect the reaction rate. With higher catalyst loading, one would expect the conversion rate for methanol to DME. However, but the amount of catalyst packing will increase the capital cost. The optimum amount of catalyst should be determined in conjunction with feed rate to the column otherwise catalyst will be a wasted. Figure 4.4 shows how the amount of catalyst loading affecting DME concentration in the top product stream. In all these simulations, the feed rate to the column was kept constant at 288 kg/h. It can be seen that the purity of the DME reaches nearly to 100 mol% when each stage in reaction zone loaded with 15 kg of catalyst.

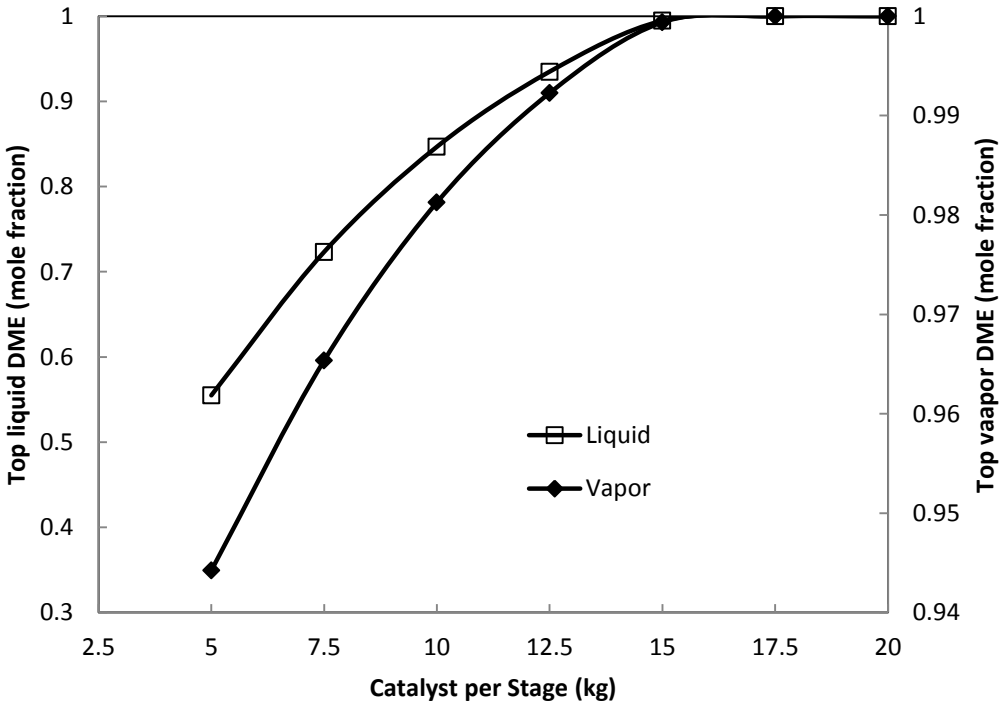

Fig 4.4 Effect of catalyst loading on DME purity.

Reaction zone sizing and placement

Reaction zone plays an important role inside a CD column, the catalyst bed inside each stage in the reaction zone acts as a small liquid-phase reactor. For highest conversion rate, the reaction zone should be placed at the middle of the column in order to give the reactant more resident time and ensure that the liquid mixture made good contact with the catalyst. After the DME and water products leave the reaction zone, enough stages for the purpose of separation are need below the reaction and rectification stages above it. Therefore, enough stages of reaction zone are needed so that catalyst are not wasted and provide enough reaction rates for the catalytic process. Figure 4.5 and Figure 4.6 show the result of adjusting the reaction zone size by changing the starting and ending stage in the column, respectively. Using a total of 13 stages of reaction zone and staring from stage 8 to stage 20 for the reaction zone gives high purity of DME in the top product stream.

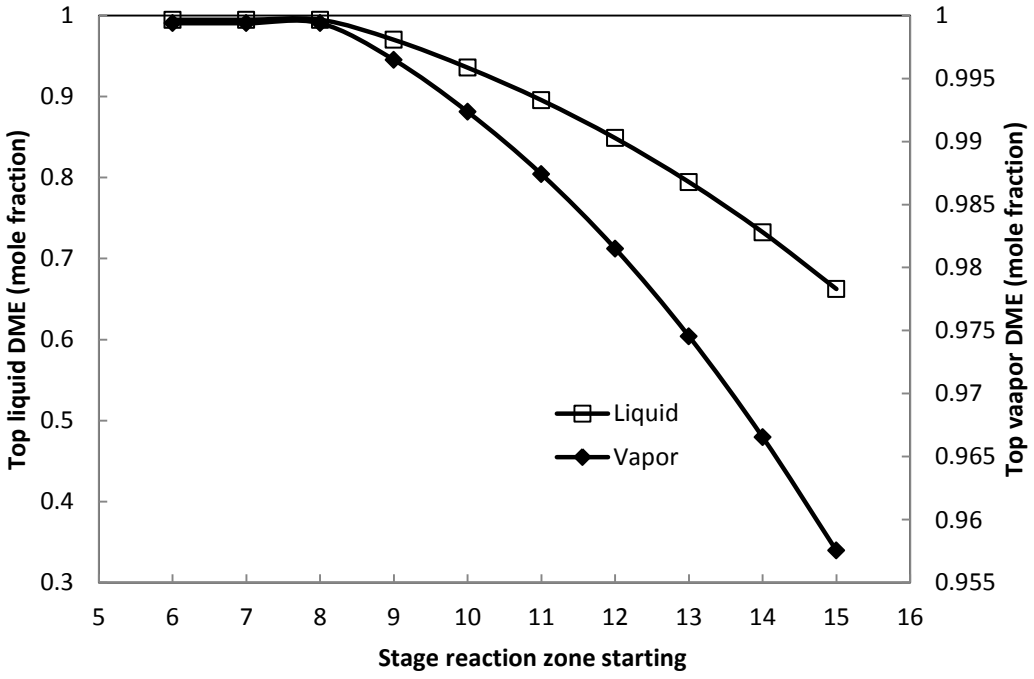

Fig 4.5 Effect of starting reaction zone stage on DME purity.

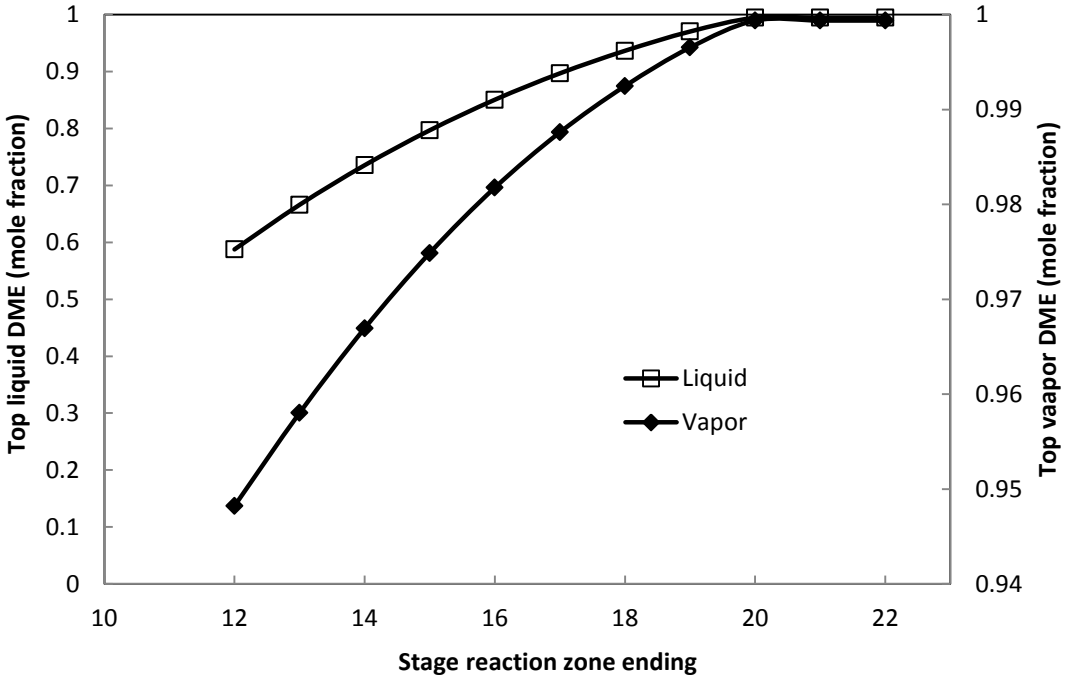

Fig 4.6 Effect of the ending reaction stage on DME purity.

Another concern of the location for the reaction zone is temperature. It is known that Amberlyst 35 has highest activity and selectivity in the temperature range of 399 to 413K. If the temperature in the catalyst bed is too high, it will cause the catalyst to deactivate leading to reduction of conversion rate and loose efficiency for the catalytic distillation column. At too low temperature the catalyst will not provide enough driving force for the reaction and will also reduce the reaction rate. Figure 4.7 shows the effect of varying reaction zone location on the temperature profile and while keeping the same size of reaction zone as well as methanol feeding at stage 8. The simulation results show that moving the reaction zone to the top of the column (i.e between stages 4-16) not only lowers the maximum temperature in the reaction zone but also lowers the conversion of the methanol to the DME in the condenser due to not enough stages for the DME to be separated. On the other hand moving the reaction zone to the lower part of the column increases the reaction zone temperature and also leads to lower concentration of DME concentration in the condenser because of not enough stripping stages for the separation. Additional simulations were preformed for

varying both the reaction zone and the feeding stage. However, it was ensure that the feeding stage was always just above reaction zone to show the effect of feeding stage on temperature profile and the purity of the DME in the top product. It can be seen from Figures 4.7 and 4.8 show very similar temperature profiles and the purity of the DME in the top product stream. It can be concluded that from our simulation results the feeding stage shows a similar result and therefore choosing the reaction zone between stages 8 to 20 is reasonable decision for the CD column in this case.

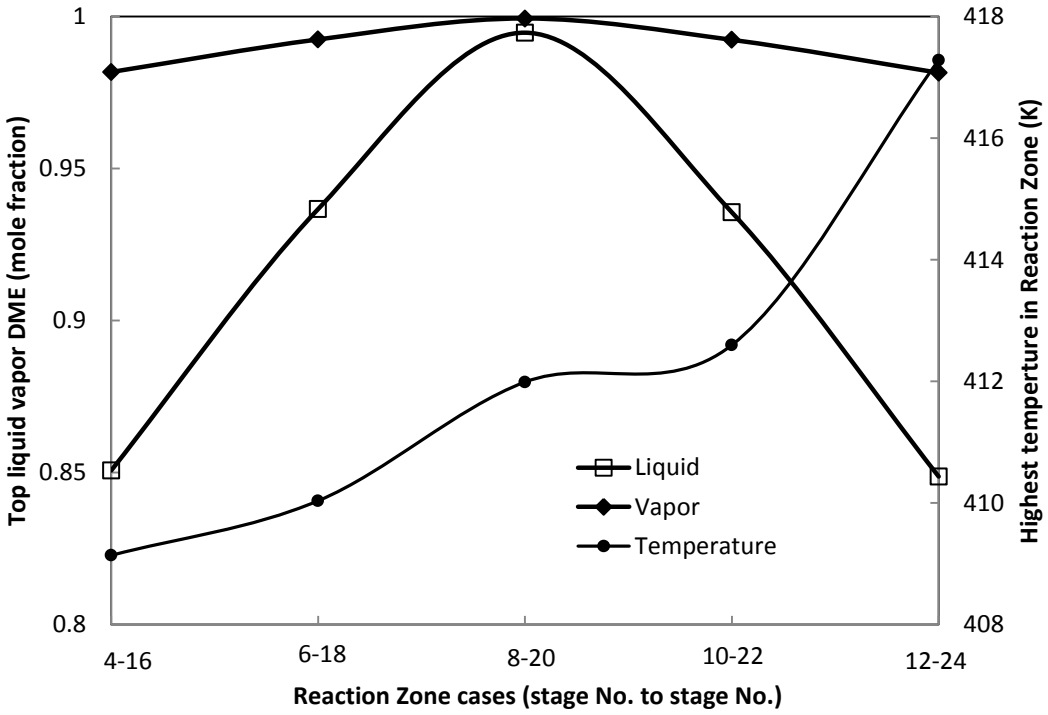

Fig 4.7 Effect of reaction zone location on temperature profile and DME purity.

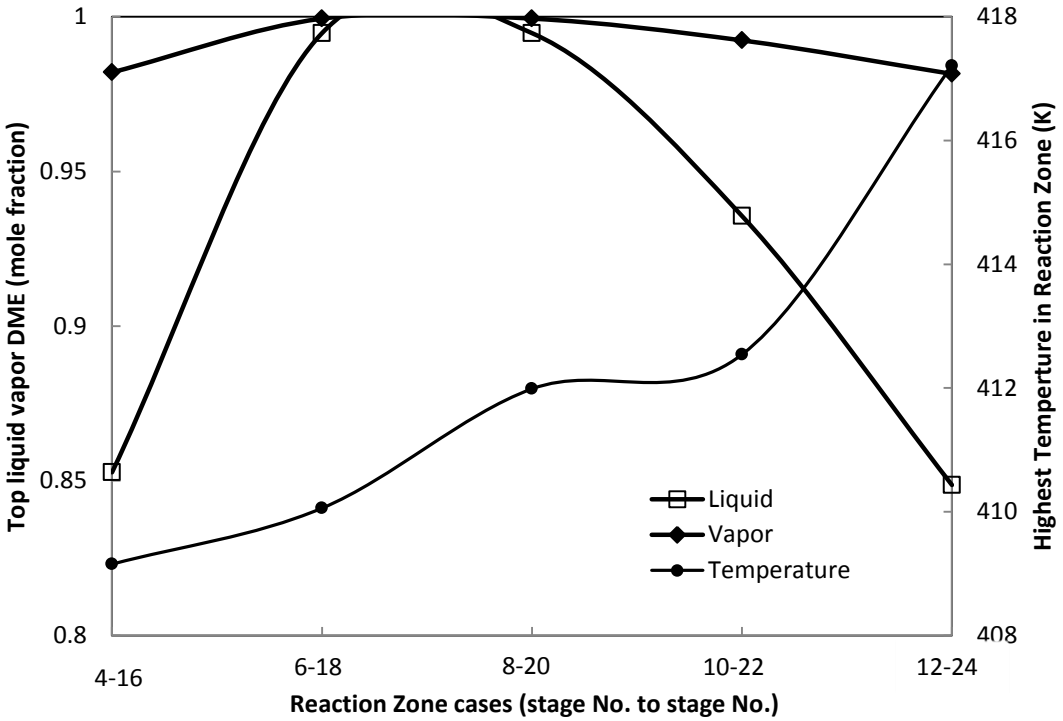

Fig 4.8 Effect of both feeding stage and reaction zone on DME purity and temperature profile.

Feed flow rate

In a CD column with a fix number of stages, reflux ratio, catalyst loading per stage and size of reaction zone can only deal with a limitation amount of methanol feed due to the capacity of liquid/vapor traffic inside the column is limited. Figure 4.9 shows the effect of increasing pure Methanol feed rate on concentration of DME in the condenser. As expected when feed rate increases more than 2.5 mole/s (288 kg/h), the purity of DME decreases. In this case the CD process is designed to operate at a limitation with pure methanol feed rate of 2.5 mole/s (288kg/h).

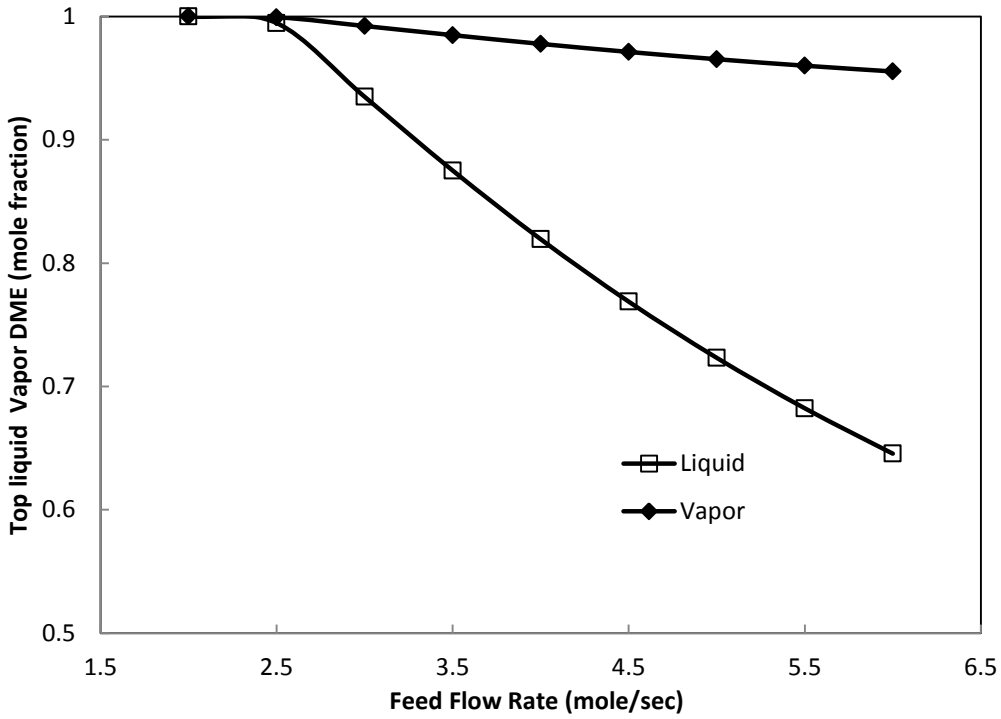

Fig 4.9 Effect of pure methanol feed flow rate on DME purity.

Methanol concentration in feed stream

Weizhu et al., (2004) and Hosseininejad et al., (2012) studies confirmed that the presence of water inhibits catalytic methanol dehydration to DME over acidic ion exchange resins. Figure 4.10 shows the effect of methanol concentration on DME and temperature profiles in the reaction zone. For these simulations, adding more water varied the methanol concentration in the feed stream. It can be seen that as the methanol concentration decreases the DME purity in the condenser decreased. Water and methanol compete for adsorption at catalytic active sites on the surface of acid catalyst, which leads to higher temperatures in the reaction zone, which leads to deactivation of the catalyst. Since methanol concentration feeding in the column affects the dehydration reaction extensively therefore goal high purity the methanol feed will be needed in order to operate the CD column to produce high purity DME.

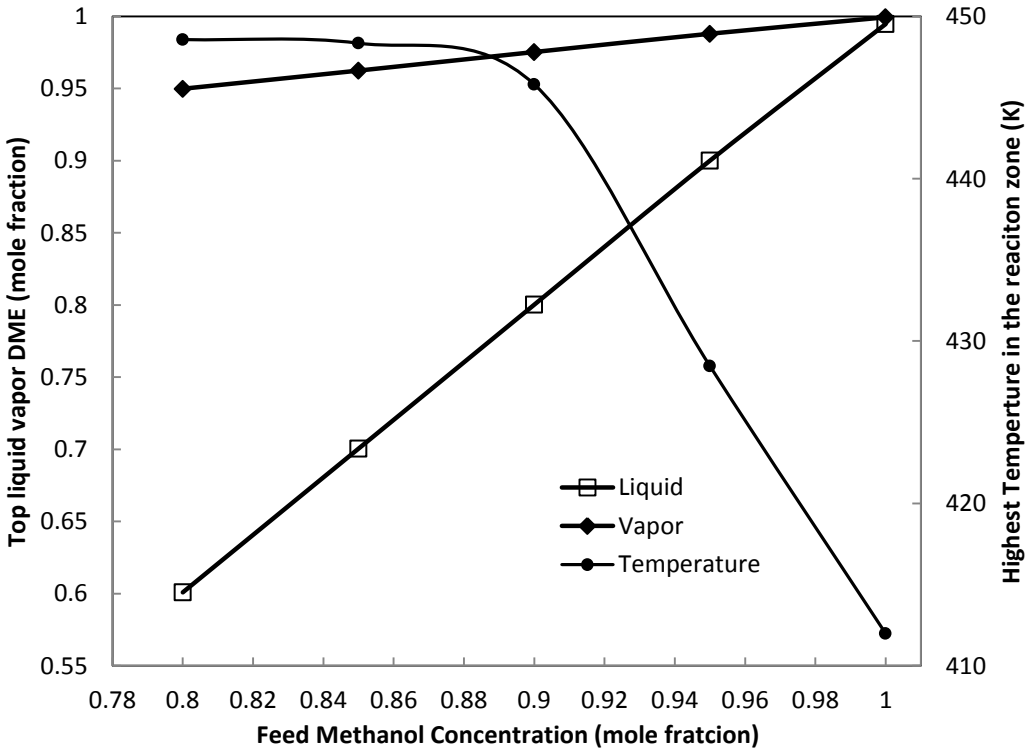

Fig 4.10 DME purity and maximum temperature in reaction zone affected by methanol feed concentration.

The summary of our parametric studies is shown in Table 4.2 and corresponding concentration and temperature profiles is shown in Figure 4.11 as obtained from the simulations. The following parameters were investigated: the total number of theoretical stages, the location of the feed stage for liquid methanol, reflux ratio, catalyst loading per stage in the reaction zone, the number of stages for the reaction zone and positioning of the reaction zone. These parameters were varied independently. It can be seen that for methanol feed flow rate of 2.5 mole/s (288 kg/h) and reflux ratio of 8, the column diameter was determined to be 0.3 m to achieve 99.99 mol% DME purity in the top product stream and produce 207.2 kg/h (164 tons/year). Each stage should be loaded with 15 kg Amberlyst 35 catalyst. Comparison of Tables 4.1 and 4.2 shown that for the same operating conditions and the same tower diameter and internals the parametric studies allowed us to reduce number of stages and reflux ratio. However, in order achieve 100% DME purity, we needed to increase catalyst load from 9.23 kg/stage to 15 kg/stage.

Table 4.2 Summary of optimized simulation design of a CD process

Feed Stream		CD Column	
Temperature	298 K	Total Stages	25
Pressure	0.9MPa	Rectification Stages	1-7
Flow rate	2.5 mol/s	Reaction stages	8-20
Feed composition	Methanol 100 mol%	Stripping stages	21-25
		Feed Stage	8
		Catalyst loading	15 kg /stage
		Catalyst bed height	0.21 m /stage
		Column pressure	0.9 MPa
		Reflux Ratio	8
		Distillate to feed ratio	0.5
		Tray type	Valve tray
		Column diameter	0.3 m.

Figure 4.11 shows that since DME is more volatile than water or methanol, and was collected in the overhead product stream and the least volatile component, water was collected at the bottom product stream. The DME concentration within the reaction zone is very low due to its high volatility. Figure 4.11 also shows that the temperature in the reaction zone (between stages 8 and 20) remains relatively constant between 400 and 410 K, which leads to prevent catalyst deactivation.

To summarize, the parametric studies results can be used to develop an optimization of design and allows us to select initial operating conditions as well as determining operating limitations. Optimization of the design includes determining such things as optimal tower diameter, tower hardware configurations and catalyst location as well as catalyst amount per stage.

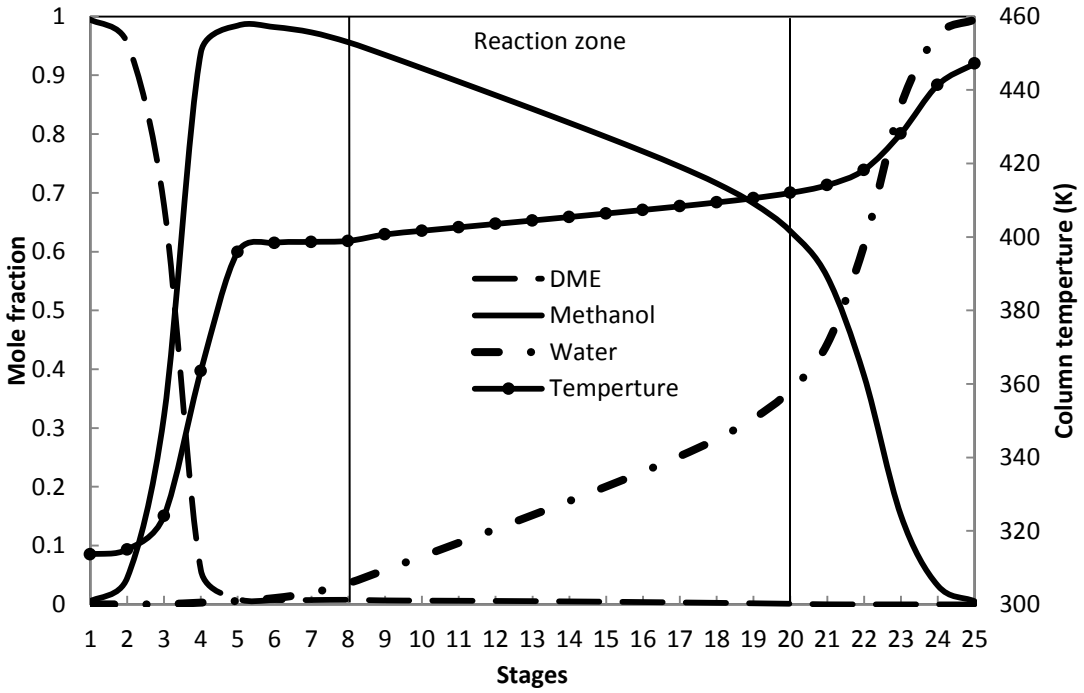

Fig 4.11 Liquid composition and temperature profiles for optimum design.

Chapter 5

Comparison between traditional DME process and CD process

Traditionally, DME has been produced from synthesis syngas via a two-step process; conversion of syngas to methanol in one reactor followed by subsequent purification of the products. Such an approach typically involves one or more chemical reactors, followed by a separation scheme, usually consisting of distillation columns and other separators. Driven by rising energy costs and increased environmental regulation on energy consumption and pollutant emission, industry is facing a need to integrate processes and improve the overall efficiency of its operations, often referred to as process intensification. Catalytic distillation can address this need for "green engineering" directly, by integrating the chemical reactor and the distillation column into a single unit operation. The objective of this chapter is to simulate the traditional DME process and catalytic distillation process and compare each process the energy requirements (i.e. operating costs).

The traditional methanol dehydration plant proposed by Haldor Topsøe's (2001) will be used as a traditional DME process. In this proposed process, the dehydration of methanol is accomplished using an acidic dehydration catalyst in a fixed bed reactor. The DME in the resulting product stream is then distilled to recover high purity DME. Finally, the waste stream from this step is further distilled in another column to recover methanol, which is recycled back to the reactor. For this process, simulation was preformed based on methanol feed stream rate of 50,000 kg/h, which are formed from syngas and to produce 333,000 Tons/year of fuel-grade DME. Figure 5.1 shows the process flow diagram of conventional methanol dehydration to DME process. A pure methanol stream first enters to a reactor to produce a mixture of 64 wt% of DME, 11 wt% of methanol and 25 wt% of water. This mixture stream is than feed to a distillation column at stage 8. This column uses 30 stages, with a diameter of 4 m and operates under pressure of 1.034 MPa. The top product stream leaving column contains 93 wt%

of DME using reflux ratio of 15. The bottom stream from the distillation column contains 19 wt% methanol, which is fed to the second distillation column to recover methanol, which is recycled back to the reactor to help produce more DME. The second distillation column has 10 stages with inner diameter of 1.4 m and operates at a pressure of 0.552 MPa. From this column, recycled methanol stream contains 61 wt% methanol using reflux ratio of 4. The diameters of both columns were determined based on vapor/liquid traffic inside each column by using ASPEN plus. Both column contained a conventional Nutter float valve trays and tray spacing was set to 0.45 m. Feed and product streams details for fixed bed reactor, main distillation column and second distillation column are given in Tables 5.1, 5.2 and 5.3, respectively.

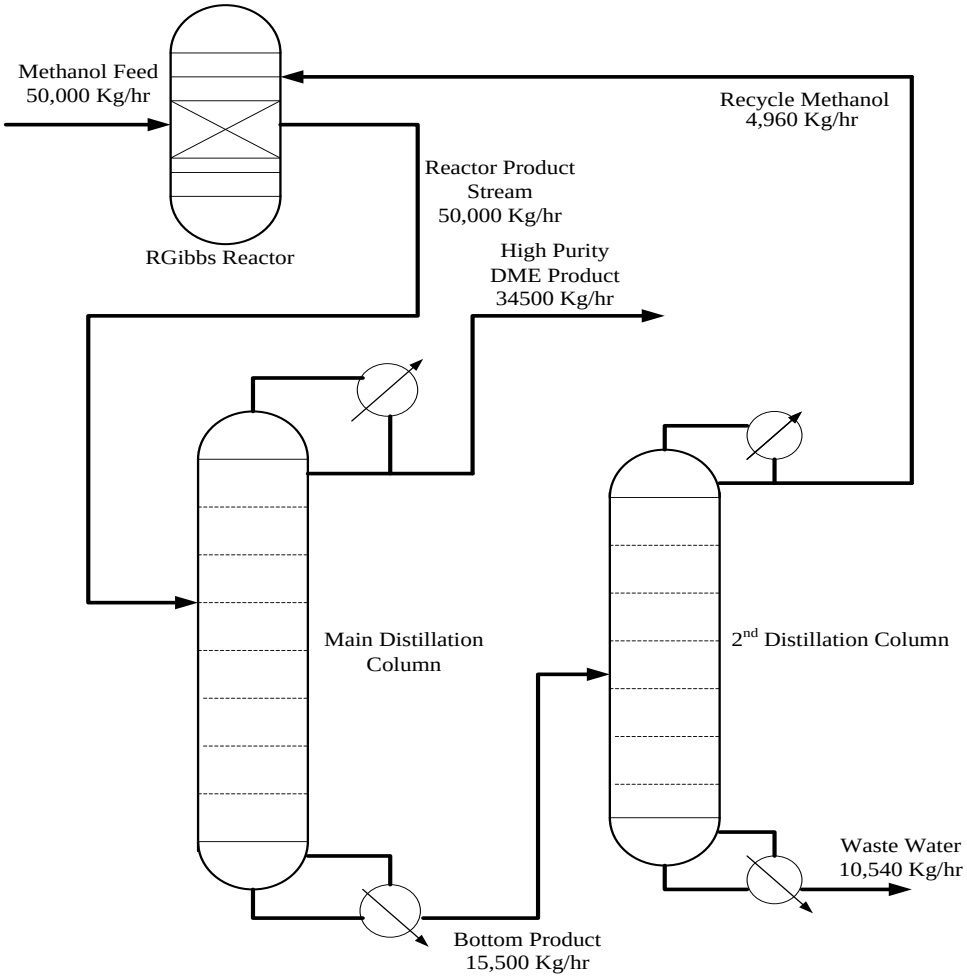

Fig 5.1 Process flow diagram for Simulation of conventional methanol dehydration to DME process.

Table 5.1. Feed and product streams detail for DME Recator.

Stream	Reactor Feed	Reactor Product	Bottom Product
Methanol (wt fraction)	1	0.11	0.07
Water (wt fraction)	0	0.25	0
DME (wt fraction)	0	0.64	0.93
Methanol flow rate (kg/h)	50,000	5,567.93	2,555.3
Water (kg/h)	0	12,490.67	3.3
DME (kg/h)	0	31,941.4	31,941.4

Table 5.2. Feed and product stream detail for the main distillation column.

Stream	Reactor Product	DME Product	Bottom Product
Methanol (wt fraction)	0.11	0.07	0.19
Water (wt fraction)	0.25	-	0.81
DME (wt fraction)	0.64	0.93	-
Methanol flow rate (kg/h)	5,567.93	2,555.3	3,012.63
Water (kg/h)	12,490.67	3.3	12,487.37
DME (kg/h)	31,941.4	31,941.4	-
Total Mass Flow (kg/h)	50,000	34,500	15,500

Table 5.3 Feed and product stream detail for the 2nd distillation column.

Stream	Bottom Product	Recycle Methanol	Waste Water
Methanol (wt fraction)	0.19	0.61	-
Water (wt fraction)	0.81	0.39	1
Methanol flow rate (kg/h)	3,012.63	3,001.47	11.17
Water (kg/h)	12,487.37	1,958.53	10,528.83
Total Mass Flow (kg/h)	15,500	4,960	10,540

Figure 5.2 shows proposed catalytic distillation process. The distillation column includes a reaction zone which contains catalyst to aid in the dehydration of methanol to DME and the separation zone, where DME would be recovered from the water and remaining methanol. The proposed catalytic distillation process is simulated to handle a feed stream of 50,000 kg/h pure methanol. It is comprised of a single catalytic reaction distillation column with 50 stages. The feed stream enters the column at stage 6. A reaction zone from stage 6 to stage 45 is designed and each stage having 900 kg Amberlyst 35 catalyst is loaded. The Langmuir-Hsinshelwood reaction kinetic is used in the reaction zone simulation. NRTL model was used for the liquid-vapor equilibrium calculation method in the simulation. Table 5.4 shows the details of the 50-stage CD column. The column diameter was set to 3.61 m based on calculation of liquid/vapor traffic in the column and a column height of 22.86 m with tray spacing of 0.45 m. The total energy that needs to be removed is 41,528.3 kW and the total energy that needs to be supplied to the process is 42,017.3 kW.

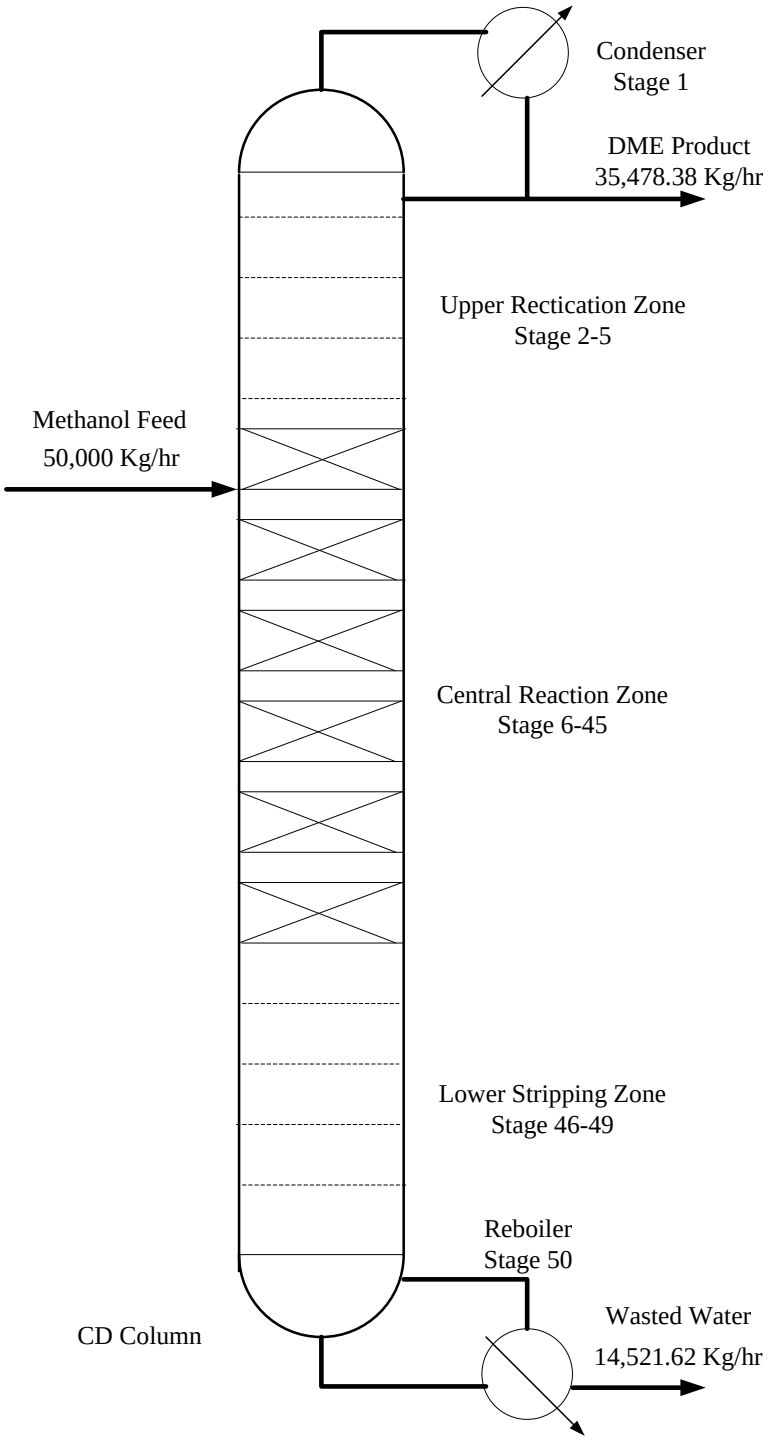

Fig 5.2 Process flow diagram for Simulation of CD process.

Table 5.4 Simulation result of block detail for CD process

Input variables	CD Column
Number of stages	50
Reaction Zone (stage-stage)	6-45
Top stage pressure (MPa)	0.81
Reflux ratio	9
Condenser heat duty (kW)	-41528.3
Reboiler heat duty (kW)	42017.3
Column Diameter (m)	3.61
Tray spacing (m)	0.456
Column Height (m)	22.86
Catalyst Loading per stage (kg)	900
Catalyst bed height per stage (m)	0.08

Table 5.5 showing simulation result details have the incoming and leaving streams for the proposed catalytic distillation column (CD). This commercializing CD process design is having a 97 wt% DME product stream producing at a rate of 342,823 tons/year. The wasted water stream contains 93 wt% of water and can be treated in to a wastewater plant directly.

Table 5.5. Simulation result of streams detail for CD process

Stream Name	Methanol Feed	DME Product	Wasted Water
Methanol (wt fraction)	1	0.03	0.07
Water (wt fraction)	0	0	0.93
DME (wt fraction)	0	0.97	0
Methanol (kg/h)	50,000	1,063.67	1,063.82
Water (kg/h)	0	0.04	13,457.8
DME (kg/h)	0	34,414.7	0
Product Mass Flow (Tones/year)	483,143	342,823	140,320

Simulating both the conventional and CD processes using the commercial simulation package Aspen Plus (version 10.10) provides details of the energy requirements to produce DME. All simulations were preformed using the NRTL model. The same feed stream was used for both cases in which it was assumed that the feed was 100% methanol with a flow rate of 50,000 kg/h. For both cases, it was assumed that vapor-liquid equilibrium was reached on all stages in all of the distillation columns. In order to make a fair comparison, the methanol dehydration reaction was determined based on the Gibbs reactor model for both processes.

Table 5.6 shows the comparison of the important parameters from both process simulations. Comparing both processes shows the advantage of the catalytic distillation column (CD) process over the traditional process for producing DME. Savings can be seen in the overall smaller plant size (i.e. capital cost) as well as the total energy requirements for heating and cooling (i.e. operating costs). The CD process produces a DME product of 97 wt%, which is higher than the traditional process's 93 wt%. This is due to the continuous removal of product from the reaction zone provides higher yield of DME

comparing to traditional pack bed reactor. Higher purity of DME has a much higher economic value in the market, further showing the benefit of the CD process. Table 5.6 also shows that the heat duty needed for operating both process is different while traditional process required 83,556.94 kW to be remove and 62,917.87 kW needed to be supplied but on the other hand, CD process only needing 41,528.3 kW to be removed and 42,017.3 kW need to be supplied.

The construction cost of both processes can only be simply estimated by amount of equipment needed. In the traditional process, a batch bed reactor and two distillation columns, main distillation column with a diameter of 4 m and height of 13.7 m and the 2^{nd} distillation column with a diameter of 1.3 m and height of 4.5 m are needed, while CD process only needing one column with a diameter of 3.6 m and height of 22.8 m. Due to the pressure needed to operate in the traditional process is higher and more columns operating, more operators are needed. Also it will be a more difficult operation and needed more control equipment in the process to monitor the columns. Therefore, the CD process has the advantage of a smaller footprint, reducing the capital cost, operating costs via energy requirements are lower and the DME product is of a higher purity.

Table 5.6 Comparison between Traditional DME process and CD process.

	Traditional DME process			CD DME process
	DME Reactor	Main Distillation Column	2nd Distillation Column	CD Column
Methanol Feed rate (kg/h)		50,000		50,000
DME Product rate (Tones/year)		333,369		342,823
DME concentration (wt%)		93		97
Total number of stages		30	10	50
Column pressure (MPa)	1.13	1.034	0.552	0.806
Column diameter (m)		4.02	1.3538	3.61
Column height (m)		13.72	4.572	22.86
Reboiler Heat Duty (kW)		53,031.7	9886.17	42,017.3
Condenser Heat Duty (kW)		-69,147.5	-10,219.5	-41,528.3
Required heat duty (kW)	-4189.94			

Chapter 6

Pilot plant scale catalytic distillation column design

The parametric studies shown in chapter 4 were preformed assuming the equilibrium stage model (i.e. NRTL model). Since all equilibrium stage models are simpler to implement and assume 100% stage efficiency, they are somewhat limited, and should be restricted to preliminary design. Furthermore, as indicated in chapter 2, the published experimental data for DME production using reactive distillation are very scares in the open literature. Therefore, the objectives of this chapter is to design and built a pilot plant scale distillation column using Aspen Plus simulation package and compare the simulation results with the experimental data to validate simulation results.

In Chapter 4, the parametric studies were preformed to obtain optimum operating condition for the column specs given in Table 4.2. Our simulations have also indicated that at higher methanol feed rate and reflux ratios the column size increased as shown in Figure 6.1. At higher methanol feed rate and reflux ratio, the liquid and vapor flows increase and consequently larger column diameters are required.

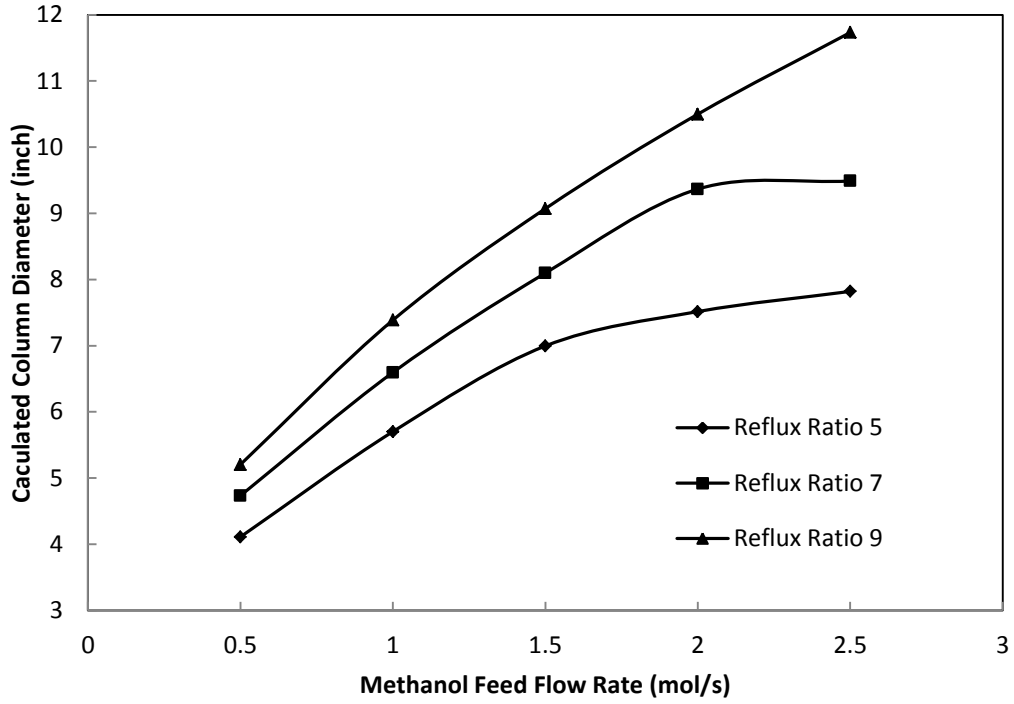

Fig 6.1 The effect of methanol feed rate and reflux ration on column diameter.

In this chapter, we will design and optimize a pilot plant scale given spec in Table 6.2. Our configuration and parametric studies indicted that methanol feed should be set to at 0.5 mole/s (57.67 kg/h), reflux ratio was selected to be 4 for producing high purity (99.81%) of DME at a 41.44 kg/h (32 tons/year) yield rate. Finally, our simulations shown that column diameter should not be more than 0.1 and having stage height minimum 1.15 m. Figure 6.2 shows corresponding liquid composition and temperature profiles for above configuration and parametric studies. Figure 6.2 shows the similar profiles as shown in Figure 4.11. Since DME is more volatile either water or methanol, and was collected in the overhead product stream and the least volatile component, water was collected at the bottom product stream. The DME concentration within the reaction zone is very low due to its high volatility. Figure 6.2 also shows that the temperature in the reaction zone (between stages 8 and 20) remains relatively constant between 400 and 410 K, which leads to prevent catalyst deactivation.

Table 6.1 Input parameters for simulation of catalytic distillation column

Feed Stream		CD Column	
Temperature	298 K	Total stages	20
Pressure	0.9MPa	Rectification stages	1-7
Feed Flow rate	0.5 mol/s	Reaction stages	7-15
Feed	Pure methanol	Stripping Stages	16-20
		Feed stage	7
		Catalyst loading	7.5 kg/Stage
		Catalyst bed height	1.03 m /stage
		Column pressure	0.9 Mpa
		Reflux ratio	4
		Distillate to feed ratio	0.5
		Tray type	Nutter float valve tray
		Column diameter	0.1 m

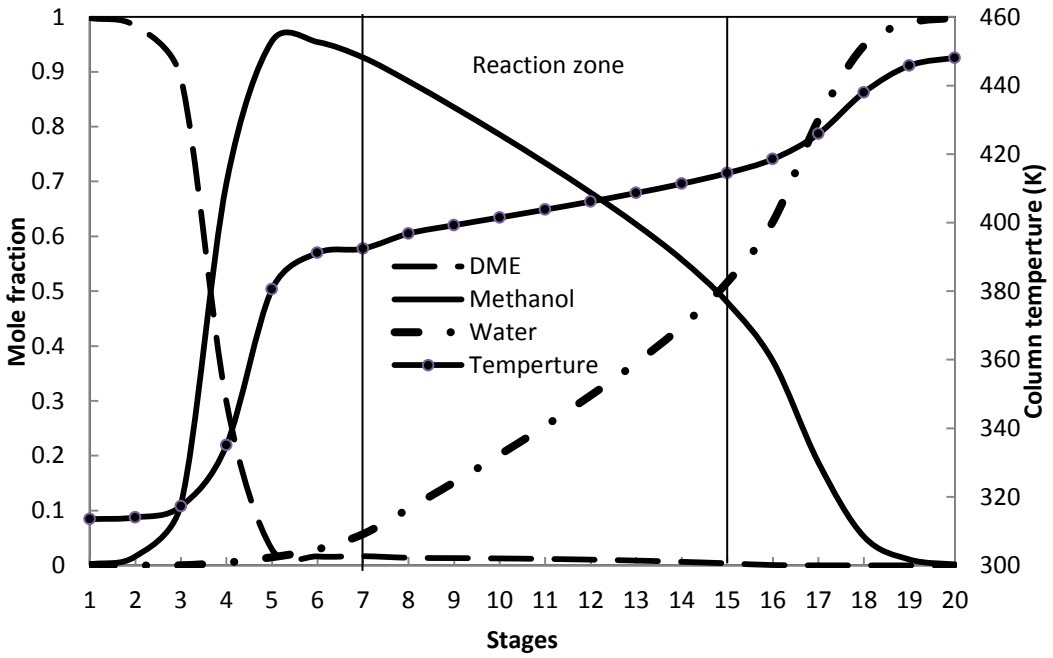

Fig 6.2 Liquid composition and temperature profiles for 4 inch column.

The accuracy of the simulation results is dependent mainly on the selection or input of valid models for vapor-liquid equilibrium in the separation zone, reaction kinetics in the reaction zone, column internals and separation efficiency. At this stage, there are no published component tray efficiency data for production of dimethyl ether from methanol using catalytic distillation column. Therefore, this pilot plant scale reactive distillation column would be used to obtain mass transfer (i.e. component tray efficiency) and hydraulic characteristics of the catalytic distillation column. The experimental data then can be used to validate simulation results and modify input models.

Chapter 7

Conclusions and Recommendations

A process using catalytic distillation for the production of dimethyl ether (DME) from methanol was simulated, by incorporating previously published kinetic models into the commercial simulation program Aspen Plus. This study focused on first developing and validating the methodology with published data and second using the developed methodology to design and optimize the catalytic distillation column internals with optimum combination of catalyst bed and separation stages for reaction and separation. Furthermore, both the conventional and catalytic distillation processes were compared using Aspen Plus simulation software to provide a clear detail of the energy requirements of both processes. The following conclusions were obtained:

- A coherent methodology was developed and confirmed by simulating a catalytic distillation process for removing acetic acid from industrial wastewater stream. The simulation results were validated qualitatively well with experimental data.
- A single catalytic distillation process was designed using the developed methodology. The simulation results shown that synthesis of high purity DME can be achieved. Furthermore, parametric studies allowed us to determine the optimum column internals with optimum combination of catalyst bed for reaction zone and separation zone as well as operating limitations.
- Finally, both conventional and catalytic distillation processes simulations indicated that there was a significant potential for reduction of overall energy requirement and capital cost for a single catalytic distillation column.

The successful designing and optimizing of a catalytic distillation process poses a number of challenges, which include the determination of appropriate reaction kinetics, all of the aspects of column selection, including column

internals design with optimum combination of catalyst bed for reaction zone and separation zone as well as operating limitations. In the open literature, there are a significant amount of experimental studies on the reaction kinetics for production of DME from methanol. However, at this stage, there are no published experimental data for DME production using catalytic distillation process. To verify the developed methodology for designing and optimizing of a catalytic distillation process, it is recommended a pilot plant scale reactive distillation column should be built to obtain mass transfer (i.e. component tray efficiency) and hydraulic characteristics of the catalytic distillation column. The experimental data then can be used to validate simulation results and modify input models.

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Appendix A

Aspen files: Removal of acetic acid by Catalytic Distillation

```
IN-UNITS SI

DEF-STREAMS CONVEN ALL

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS MASS-BAL-CHE=YES PARADIGM=SM OLD-DATABANK=YES

DATABANKS       PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  NOASPENPCD

PROP-SOURCES    PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
   MEAC         C3H6O2-3 /
   MEOH         CH4O /
   WATER        H2O /
   HAC          C2H4O2-1

FLOWSHEET
   BLOCK        B1       IN=F1 F2          OUT=3 4

PROPERTIES NRTL
   PROPERTIES NRTL-2 / NRTL-HOC
PROP-DATA HOCETA-1
   IN-UNITS     SI
   PROP-LIST    HOCETA
   BPVAL        MEAC    MEAC    .8500000000
   BPVAL        MEAC    MEOH    1.300000000
   BPVAL        MEAC    WATER   1.300000000
   BPVAL        MEAC    HAC     2.000000000
   BPVAL        MEOH    MEAC    1.300000000
   BPVAL        MEOH    MEOH    1.630000000
   BPVAL        MEOH    WATER   1.550000000
   BPVAL        MEOH    HAC     2.500000000
   BPVAL        WATER   MEAC    1.300000000
   BPVAL        WATER   MEOH    1.550000000
   BPVAL        WATER   WATER   1.700000000
   BPVAL        WATER   HAC     2.500000000
   BPVAL        HAC     MEAC    2.000000000
   BPVAL        HAC     MEOH    2.500000000
   BPVAL        HAC     WATER   2.500000000
   BPVAL        HAC     HAC     4.500000000
PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL MEAC MEOH 0.0 422.7587966 .3000000000 0.0 0.0 0.0  &
     70.70000343 148.1000028
```

```
  BPVAL MEOH MEAC 0.0 234.9084581 .3000000000 0.0 0.0 0.0  &
    70.70000343 148.1000028
  BPVAL MEAC WATER -2.929700000 2242.107522 .3500000000 0.0  &
    0.0 0.0 77.00000338 194.0000024
  BPVAL WATER MEAC 3.522200000 -552.9646756 .3500000000 0.0  &
    0.0 0.0 77.00000338 194.0000024
  BPVAL MEOH WATER -.6930000000 311.3767775 .3000000000 0.0  &
    0.0 0.0 76.98200338 212.0000023
  BPVAL WATER MEOH 2.732200000 -1111.083651 .3000000000 0.0  &
    0.0 0.0 76.98200338 212.0000023
  BPVAL MEOH HAC 0.0 -606.2554751 .3000000000 0.0 0.0 0.0  &
    113.0000031 113.0000031
  BPVAL HAC MEOH 0.0 356.3600371 .3000000000 0.0 0.0 0.0  &
    113.0000031 113.0000031

PROP-DATA NRTL-2
  IN-UNITS SI
  PROP-LIST NRTL 2
  BPVAL MEAC MEOH 0.0 234.8660000 .3000000000 0.0 0.0 0.0  &
    294.6500000 337.6500000
  BPVAL MEOH MEAC 0.0 130.5047000 .3000000000 0.0 0.0 0.0  &
    294.6500000 337.6500000
  BPVAL MEAC WATER -2.929700000 1245.615300 .3500000000 0.0  &
    0.0 0.0 298.1500000 363.1500000
  BPVAL WATER MEAC 3.522200000 -307.2026000 .3500000000 0.0  &
    0.0 0.0 298.1500000 363.1500000
  BPVAL MEOH WATER -.6930000000 172.9871000 .3000000000 0.0  &
    0.0 0.0 298.1400000 373.1500000
  BPVAL WATER MEOH 2.732200000 -617.2687000 .3000000000 0.0  &
    0.0 0.0 298.1400000 373.1500000
  BPVAL MEOH HAC 0.0 -336.8086000 .3000000000 0.0 0.0 0.0  &
    318.1500000 318.1500000
  BPVAL HAC MEOH 0.0 197.9778000 .3000000000 0.0 0.0 0.0  &
    318.1500000 318.1500000

STREAM F1
  IN-UNITS ENG
  SUBSTREAM MIXED       TEMP=70. <C>     PRES=0.95 <bar>  MASS-FLOW=140. <gm/min>
  MASS-FRAC      MEAC 0. / MEOH 0. / WATER 0.9008 / HAC  0.0992

STREAM F2
  SUBSTREAM MIXED TEMP=50. <C> PRES=0.95 <bar>
  MASS-FLOW      MEAC 0. <gm/min> / MEOH 27.5 <gm/min> /
                 WATER  0. <gm/min> / HAC 0. <gm/min>



BLOCK B1 RADFRAC
  IN-UNITS ENG
  PARAM NSTAGE=15 EFF=MURPHREE
  COL-CONFIG CONDENSER=TOTAL
  RATESEP-ENAB CALC-MODE=EQUILIBRIUM
```

```
  FEEDS F1 4 / F2 12
  PRODUCTS 3 1 L / 4 15 L
  P-SPEC 1 0.935 <bar>
  COL-SPECS MASS-D=17.54 <gm/min> MASS-L1=153.5 <gm/min>
  COMP-EFF 1 MEAC 0.0001 / 1 MEOH 0.0001 / 1 WATER  &
    0.0001 / 1 HAC 0.0001 / 2 MEAC 0.7 / 2 MEOH 0.75 / &
    2 WATER 0.75 / 2 HAC 0.7 / 3 MEAC 0.0001 / 3  &
    MEOH 0.0001 / 3 WATER 0.0001 / 3 HAC 0.0001 / 4  &
    MEAC 0.7 / 4 MEOH 0.8 / 4 WATER 0.75 / 4 HAC  &
    0.75 / 5 MEAC 0.0001 / 5 MEOH 0.0001 / 5 WATER  &
    0.0001 / 5 HAC 0.0001 / 6 MEAC 0.9 / 6 MEOH 1.05 / &
    6 WATER 1.05 / 6 HAC 0.75 / 7 MEAC 0.0001 / 7  &
    MEOH 0.0001 / 7 WATER 0.0001 / 7 HAC 0.0001 / 8  &
    MEAC 0.9 / 8 MEOH 1.05 / 8 WATER 1.05 / 8 HAC  &
    0.74 / 9 MEAC 0.0001 / 9 MEOH 0.0001 / 9 WATER  &
    0.0001 / 9 HAC 0.0001 / 10 MEAC 0.9 / 10 MEOH  &
    1.05 / 10 WATER 1.05 / 10 HAC 0.75 / 11 MEAC  &
    0.0001 / 11 MEOH 0.0001 / 11 WATER 0.0001 / 11  &
    HAC 0.0001 / 12 MEAC 0.9 / 12 MEOH 1.05 / 12  &
    WATER 1.05 / 12 HAC 0.72 / 13 MEAC 0.0001 / 13  &
    MEOH 0.0001 / 13 WATER 0.0001 / 13 HAC 0.0001 /  &
    14 MEAC 0.9 / 14 MEOH 1.05 / 14 WATER 1.05 / 14  &
    HAC 0.75 / 15 MEAC 0.0001 / 15 MEOH 0.0001 / 15  &
    WATER 0.0001 / 15 HAC 0.0001
  REAC-STAGES 5 5 R-1 / 7 7 R-1 / 9 9 R-1 / 11 11  &
    R-1 / 13 13 R-1
  HOLD-UP 5 5 VOL-LHLDP=0.027 <cum> / 7 7  &
    VOL-LHLDP=0.027 <cum> / 9 9 VOL-LHLDP=0.027 <cum> / 11  &
    11 VOL-LHLDP=0.027 <cum> / 13 13 VOL-LHLDP=0.027 <cum>
  TRAY-REPORT TRAY-OPTION=ALL-TRAYS

EO-CONV-OPTI

BLOCK-REPORT COMPBAL

STREAM-REPOR MOLEFLOW MOLEFRAC

REACTIONS R-1 REAC-DIST
  PARAM SUBROUTINE=RN2
  REAC-DATA 1 KINETIC
  STOIC 1 MEOH -1. / HAC -1. / WATER 1. / MEAC 1.
```

User define kinetic subroutine fortran file

```
SUBROUTINE  RN2          (N,    NCOMP,  NR,    NRL,    NRV,
   2                     T,    TLIQ,   TVAP,  P,      PHFRAC,
   3                     F,    X,      Y,     IDX,    NBOPST,
   4                     KDIAG,  STOIC,  IHLBAS, HLDLIQ,  TIMLIQ,
   5                     IHVBAS, HLDVAP,  TIMVAP, NINT,   INT,
   6                     NREAL,  REAL,   RATES,  RATEL,   RATEV,
   7                     NINTB,  INTB,   NREALB, REALB,   NIWORK,
   8                     IWORK,  NWORK,  WORK)

    INTEGER IMISS
    REAL*8 REAL(NREAL),  RMISS
    REAL*8 Rate, X1, X2, X3, X4

    X1=X(1,3)
    X2=X(2,3)
    X3=X(3,3)
    X4=X(4,3)
    RATE=HLDLIQ*4.2*10**9*
   & EXP(-58500.0/(8.314*T))*
   & (X2*X4-X3*X1/(6.39-0.012*(T-273.15)))

    RATES(1) = RATE
    RATES(2) = -RATE
    RATES(3) = RATE
    RATES(4) = -RATE

    RETURN
    END
```

CATALYTIC DISTILLATION
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
F2	----	B1	F1	----	B1
3	B1	----	4	B1	----

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
B1	F1 F2	3 4

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:B1

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS(KMOL/SEC)				
MEAC	0.00000	0.314632E-05	0.314632E-05	0.217203E-09
MEOH	0.143041E-04	0.111578E-04	-0.314632E-05	-0.477772E-10
WATER	0.116671E-03	0.119818E-03	0.314632E-05	0.570352E-11
HAC	0.385440E-05	0.708083E-06	-0.314632E-05	-0.177303E-09
TOTAL BALANCE				
MOLE(KMOL/SEC)	0.134830E-03	0.134830E-03	0.00000	-0.402063E-15
MASS(KG/SEC)	0.279167E-02	0.279167E-02		-0.621393E-15
ENTHALPY(WATT)	-38074.0	-37996.8		-0.202999E-02

CATALYTIC DISTILLATION

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
MEAC	C	C3H6O2-3	METHYL-ACETATE
MEOH	C	CH4O	METHANOL
WATER	C	H2O	WATER
HAC	C	C2H4O2-1	ACETIC-ACID

CATALYTIC DISTILLATION
U-O-S BLOCK SECTION

BLOCK: B1 MODEL: RADFRAC

INLETS	- F1	STAGE	4
	F2	STAGE	12
OUTLETS	- 3	STAGE	1
	4	STAGE	15

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL				
COMPONENTS(KMOL/SEC)				
MEAC	0.00000	0.314632E-05	0.314632E-05	0.217203E-09
MEOH	0.143041E-04	0.111578E-04	-0.314632E-05	-0.477772E-10
WATER	0.116671E-03	0.119818E-03	0.314632E-05	0.570352E-11
HAC	0.385440E-05	0.708083E-06	-0.314632E-05	-0.177303E-09
TOTAL BALANCE				
MOLE(KMOL/SEC)	0.134830E-03	0.134830E-03	0.00000	-0.402063E-15
MASS(KG/SEC)	0.279167E-02	0.279167E-02		-0.621393E-15
ENTHALPY(WATT)	-38074.0	-37996.8		-0.202999E-02

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	15
ALGORITHM OPTION	STANDARD
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST		0.0
MASS REFLUX RATE	KG/SEC	0.0025583
MASS DISTILLATE RATE	KG/SEC	0.00029233

**** REAC-STAGES SPECIFICATIONS ****

STAGE	TO STAGE	REACTIONS/CHEMISTRY ID
5	5	R-1
7	7	R-1
9	9	R-1
11	11	R-1
13	13	R-1

**** HOLD-UP SPECIFICATIONS ****

STAGE	TO STAGE	LIQUID HOLDUP	VAPOR HOLDUP
5	5	2.7000-02 CUM	MISSING
7	7	2.7000-02 CUM	MISSING
9	9	2.7000-02 CUM	MISSING
11	11	2.7000-02 CUM	MISSING
13	13	2.7000-02 CUM	MISSING

***** REACTION PARAGRAPH R-1 *****

**** REACTION PARAMETERS ****

RXN NO.	TYPE	PHASE	CONC. BASIS	TEMP APP TO EQUIL K	CONVERSION
1	KINETIC	LIQUID	MOLAR		

** STOICHIOMETRIC COEFFICIENTS **

RXN NO.	MEAC	MEOH	WATER	HAC
1	1.000	-1.000	1.000	-1.000

**** PROFILES ****

P-SPEC STAGE 1 PRES, N/SQM 93,500.0

**** COMPONENT MURPHREE EFFICIENCY ****

STAGE	MEAC	MEOH	WATER	HAC
1	1.0000-04	1.0000-04	1.0000-04	1.0000-04
2	0.7000	0.7500	0.7500	0.7000
3	1.0000-04	1.0000-04	1.0000-04	1.0000-04
4	0.7000	0.8000	0.7500	0.7500
5	1.0000-04	1.0000-04	1.0000-04	1.0000-04
6	0.9000	1.0500	1.0500	0.7500
7	1.0000-04	1.0000-04	1.0000-04	1.0000-04
8	0.9000	1.0500	1.0500	0.7400
9	1.0000-04	1.0000-04	1.0000-04	1.0000-04
10	0.9000	1.0500	1.0500	0.7500
11	1.0000-04	1.0000-04	1.0000-04	1.0000-04
12	0.9000	1.0500	1.0500	0.7200
13	1.0000-04	1.0000-04	1.0000-04	1.0000-04
14	0.9000	1.0500	1.0500	0.7500
15	1.0000-04	1.0000-04	1.0000-04	1.0000-04

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	3	4
COMPONENT:		
MEAC	.99668	.33181E-02
MEOH	.11768	.88232
WATER	.80638E-02	.99194
HAC	.12941E-01	.98706

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	K	326.821
BOTTOM STAGE TEMPERATURE	K	360.869
TOP STAGE LIQUID FLOW	KMOL/SEC	0.474701-04
BOTTOM STAGE LIQUID FLOW	KMOL/SEC	0.00012941
TOP STAGE VAPOR FLOW	KMOL/SEC	0.0
BOILUP VAPOR FLOW	KMOL/SEC	0.445882-04
MOLAR REFLUX RATIO		8.75143
MOLAR BOILUP RATIO		0.34456
CONDENSER DUTY (W/O SUBCOOL)	WATT	-1,757.78
REBOILER DUTY	WATT	1,835.07

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.24023E-07	STAGE= 3
BUBBLE POINT	0.19343E-06	STAGE= 2
COMPONENT MASS BALANCE	0.14532E-09	STAGE= 9 COMP=HAC
ENERGY BALANCE	0.67284E-07	STAGE= 2

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE K	PRESSURE N/SQM	ENTHALPY J/KMOL LIQUID	ENTHALPY J/KMOL VAPOR	HEAT DUTY WATT
1	326.82	93500.	-0.36167E+09	-0.32863E+09	-1757.7795
2	329.53	93500.	-0.32413E+09	-0.32844E+09	
3	329.00	93500.	-0.32405E+09	-0.29284E+09	
4	345.96	93500.	-0.28579E+09	-0.29184E+09	
5	347.02	93500.	-0.28558E+09	-0.25186E+09	
6	353.80	93500.	-0.28206E+09	-0.25152E+09	
7	349.78	93500.	-0.28269E+09	-0.24093E+09	
8	354.93	93500.	-0.27985E+09	-0.24068E+09	
9	351.59	93500.	-0.28042E+09	-0.23234E+09	
10	354.66	93500.	-0.27766E+09	-0.23220E+09	
11	352.13	93500.	-0.27814E+09	-0.22396E+09	
12	352.53	93500.	-0.27433E+09	-0.22394E+09	
13	350.99	93500.	-0.27465E+09	-0.22270E+09	
14	355.17	93500.	-0.27547E+09	-0.22252E+09	
15	360.87	93500.	-0.27847E+09	-0.22563E+09	1835.0695

STAGE	FLOW RATE KMOL/SEC		FEED RATE KMOL/SEC			PRODUCT RATE KMOL/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5289E-04	0.000				.54243-05	
2	0.4425E-04	0.5289E-04					
3	0.4281E-04	0.4968E-04					
4	0.1623E-03	0.4823E-04	.12053-03				
5	0.1628E-03	0.4718E-04					
6	0.1644E-03	0.4770E-04					
7	0.1617E-03	0.4934E-04					
8	0.1632E-03	0.4659E-04					
9	0.1611E-03	0.4806E-04					
10	0.1623E-03	0.4600E-04					
11	0.1609E-03	0.4724E-04					
12	0.1753E-03	0.4577E-04	.14304-04				
13	0.1741E-03	0.4589E-04					
14	0.1740E-03	0.4466E-04					
15	0.1294E-03	0.4459E-04				.12941-03	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KMOL/SEC		FEED RATE KMOL/SEC			PRODUCT RATE KMOL/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.2851E-02	0.000				.29233-03	
2	0.1828E-02	0.2851E-02					
3	0.1767E-02	0.2121E-02					
4	0.3580E-02	0.2059E-02	.23333-02				
5	0.3597E-02	0.1539E-02					
6	0.3515E-02	0.1556E-02					
7	0.3433E-02	0.1474E-02					
8	0.3403E-02	0.1392E-02					
9	0.3345E-02	0.1362E-02					
10	0.3366E-02	0.1304E-02					
11	0.3325E-02	0.1325E-02					
12	0.3712E-02	0.1284E-02	.45833-03				
13	0.3679E-02	0.1212E-02					
14	0.3539E-02	0.1180E-02					
15	0.2499E-02	0.1040E-02				.24993-02	

**** MOLE-X-PROFILE ****

STAGE	MEAC	MEOH	WATER	HAC
1	0.57812	0.24207	0.17812	0.16893E-02
2	0.34367	0.27155	0.37941	0.53591E-02
3	0.34278	0.27167	0.38018	0.53732E-02
4	0.26714E-01	0.10468	0.84296	0.25646E-01
5	0.22203E-01	0.11050	0.83678	0.30509E-01
6	0.71222E-02	0.12235	0.84085	0.29677E-01
7	0.14524E-01	0.10829	0.85613	0.21055E-01
8	0.42569E-02	0.12454	0.85080	0.20402E-01
9	0.10048E-01	0.11360	0.86231	0.14038E-01
10	0.27964E-02	0.14211	0.84154	0.13559E-01
11	0.74151E-02	0.13341	0.85046	0.87106E-02
12	0.20726E-02	0.19313	0.79688	0.79156E-02
13	0.55338E-02	0.18730	0.80281	0.43625E-02
14	0.90203E-03	0.14870	0.84590	0.45035E-02
15	0.80674E-04	0.76076E-01	0.91844	0.54010E-02

**** MOLE-Y-PROFILE ****

STAGE	MEAC	MEOH	WATER	HAC
1	0.57813	0.24207	0.17811	0.16891E-02
2	0.57812	0.24207	0.17812	0.16893E-02
3	0.36927	0.26833	0.35743	0.49584E-02
4	0.36924	0.26834	0.35746	0.49589E-02
5	0.15836	0.38789	0.44704	0.67115E-02
6	0.15833	0.38791	0.44705	0.67117E-02
7	0.10354	0.41817	0.47356	0.47300E-02
8	0.10352	0.41818	0.47356	0.47300E-02
9	0.65940E-01	0.46385	0.46720	0.30109E-02
10	0.65923E-01	0.46387	0.46720	0.30109E-02
11	0.39534E-01	0.55260	0.40621	0.16569E-02
12	0.39521E-01	0.55262	0.40620	0.16569E-02

13	0.21342E-01	0.50954	0.46777	0.13535E-02
14	0.21333E-01	0.50954	0.46778	0.13536E-02
15	0.32858E-02	0.35945	0.63536	0.18987E-02

**** K-VALUES ****

STAGE	MEAC	MEOH	WATER	HAC
1	1.2016	0.94821	0.42517	0.53634E-01
2	1.9426	0.85918	0.31194	0.53788E-01
3	1.9140	0.83976	0.30386	0.52468E-01
4	17.206	2.2779	0.38863	0.17058
5	17.644	2.3784	0.40622	0.18083
6	23.086	3.1822	0.53316	0.24842
7	21.422	2.7467	0.45207	0.20796
8	25.300	3.3753	0.55625	0.26145
9	23.742	2.9882	0.48568	0.22603
10	24.622	3.2940	0.55172	0.25534
11	23.454	3.0040	0.49775	0.22858
12	20.043	2.8507	0.51342	0.22422
13	19.420	2.6944	0.48200	0.20920
14	25.873	3.3787	0.56243	0.26021
15	40.729	4.7249	0.69178	0.35154

**** RATES OF GENERATION ****
KMOL/SEC

STAGE	MEAC	MEOH	WATER	HAC
1	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000
3	0.000	0.000	0.000	0.000
4	0.000	0.000	0.000	0.000
5	-.8013E-06	0.8013E-06	-.8013E-06	0.8013E-06
6	0.000	0.000	0.000	0.000
7	0.1462E-05	-.1462E-05	0.1462E-05	-.1462E-05
8	0.000	0.000	0.000	0.000
9	0.1061E-05	-.1061E-05	0.1061E-05	-.1061E-05
10	0.000	0.000	0.000	0.000
11	0.7975E-06	-.7975E-06	0.7975E-06	-.7975E-06
12	0.000	0.000	0.000	0.000
13	0.6266E-06	-.6266E-06	0.6266E-06	-.6266E-06
14	0.000	0.000	0.000	0.000
15	0.000	0.000	0.000	0.000

**** MASS-X-PROFILE ****

STAGE	MEAC	MEOH	WATER	HAC
1	0.79465	0.14392	0.59542E-01	0.18824E-02
2	0.61619	0.21059	0.16543	0.77892E-02
3	0.61529	0.21093	0.16596	0.78188E-02
4	0.89710E-01	0.15205	0.68842	0.69817E-01
5	0.74449E-01	0.16027	0.68235	0.82929E-01
6	0.24680E-01	0.18338	0.70857	0.83363E-01
7	0.50672E-01	0.16341	0.72637	0.59548E-01
8	0.15118E-01	0.19131	0.73483	0.58737E-01
9	0.35850E-01	0.17532	0.74822	0.40603E-01

10	0.99906E-02	0.21959	0.73114	0.39270E-01
11	0.26577E-01	0.20683	0.74129	0.25309E-01
12	0.72513E-02	0.29227	0.67803	0.22451E-01
13	0.19395E-01	0.28394	0.68427	0.12395E-01
14	0.32851E-02	0.23423	0.74919	0.13296E-01
15	0.30943E-03	0.12621	0.85669	0.16793E-01

**** MASS-Y-PROFILE ****

STAGE	MEAC	MEOH	WATER	HAC
1	0.79466	0.14392	0.59538E-01	0.18822E-02
2	0.79465	0.14392	0.59542E-01	0.18824E-02
3	0.64079	0.20140	0.15084	0.69750E-02
4	0.64076	0.20141	0.15085	0.69759E-02
5	0.35966	0.38106	0.24692	0.12357E-01
6	0.35962	0.38109	0.24693	0.12358E-01
7	0.25666	0.44836	0.28547	0.95047E-02
8	0.25662	0.44839	0.28549	0.95051E-02
9	0.17233	0.52435	0.29694	0.63789E-02
10	0.17229	0.52438	0.29695	0.63791E-02
11	0.10440	0.63119	0.26086	0.35470E-02
12	0.10437	0.63122	0.26087	0.35470E-02
13	0.59849E-01	0.61806	0.31901	0.30770E-02
14	0.59826E-01	0.61807	0.31902	0.30772E-02
15	0.10437E-01	0.49387	0.49081	0.48891E-02

**** MURPHREE EFF ****

STAGE	MEAC	MEOH	WATER	HAC
1	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
2	0.70000	0.75000	0.75000	0.70000
3	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
4	0.70000	0.80000	0.75000	0.75000
5	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
6	0.90000	1.0500	1.0500	0.75000
7	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
8	0.90000	1.0500	1.0500	0.74000
9	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
10	0.90000	1.0500	1.0500	0.75000
11	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
12	0.90000	1.0500	1.0500	0.72000
13	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03
14	0.90000	1.0500	1.0500	0.75000
15	0.10000E-03	0.10000E-03	0.10000E-03	0.10000E-03

CATALYTIC DISTILLATION
STREAM SECTION

STREAM ID	3	4	F1	F2
FROM :	B1	B1	----	----
TO :	----	----	B1	B1
SUBSTREAM: MIXED				
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/SEC				
MEAC	3.1359-06	1.0440-08	0.0	0.0
MEOH	1.3130-06	9.8447-06	0.0	1.4304-05
WATER	9.6619-07	1.1885-04	1.1667-04	0.0
HAC	9.1633-09	6.9892-07	3.8544-06	0.0
COMPONENTS: MOLE FRAC				
MEAC	0.5781	8.0674-05	0.0	0.0
MEOH	0.2421	7.6076-02	0.0	1.0000
WATER	0.1781	0.9184	0.9680	0.0
HAC	1.6893-03	5.4010-03	3.1980-02	0.0
TOTAL FLOW:				
KMOL/SEC	5.4243-06	1.2941-04	1.2053-04	1.4304-05
KG/SEC	2.9233-04	2.4993-03	2.3333-03	4.5833-04
CUM/SEC	3.2957-07	2.7928-06	2.4736-06	6.0112-07
STATE VARIABLES:				
TEMP K	326.8213	360.8695	343.1500	323.1500
PRES N/SQM	9.3500+04	9.3500+04	9.5000+04	9.5000+04
VFRAC	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0
ENTHALPY:				
J/KMOL	-3.6167+08	-2.7847+08	-2.8790+08	-2.3593+08
J/KG	-6.7109+06	-1.4418+07	-1.4871+07	-7.3630+06
WATT	-1961.8122	-3.6035+04	-3.4699+04	-3374.7102
ENTROPY:				
J/KMOL-K	-2.9519+05	-1.5329+05	-1.5424+05	-2.3266+05
J/KG-K	-5477.2767	-7936.9300	-7966.9449	-7260.9935
DENSITY:				
KMOL/CUM	16.4585	46.3348	48.7257	23.7957
KG/CUM	887.0067	894.9092	943.3120	762.4658
AVG MW	53.8935	19.3140	19.3596	32.0422

BLOCK STATUS

```
 ************************************************************************
*                                                                        *
* Calculations were completed normally                                   *
*                                                                        *
* All Unit Operation blocks were completed normally                      *
*                                                                        *
* All streams were flashed normally                                      *
*                                                                        *
************************************************************************
```

Appendix B

Aspen files: DME CD process of Eley-Rideal model

```
DYNAMICS
   DYNAMICS RESULTS=ON

IN-UNITS SI MOLE-FLOW='mol/sec' MOLES=mol

DEF-STREAMS CONVEN ALL

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS MASS-BAL-CHE=YES OLD-DATABANK=YES

DATABANKS PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      NOASPENPCD

PROP-SOURCES PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
   WATER H2O /
   METHANOL CH4O /
   DIMET-01 C2H6O-1

FLOWSHEET
   BLOCK B1 IN=1 OUT=2 3

PROPERTIES NRTL
   PROPERTIES IDEAL / NRTL-SAC
PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL WATER METHANOL 2.732200000 -1111.083651 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL WATER -.6930000000 311.3767775 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL DIMET-01 0.0 1175.411331 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374
   BPVAL DIMET-01 METHANOL 0.0 -34.08695973 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374

STREAM 1
   IN-UNITS ENG
   SUBSTREAM MIXED TEMP=298. <K> PRES=0.9 <MPa>  &
      MOLE-FLOW=2.5 <mol/sec>
   MOLE-FLOW METHANOL 1.

BLOCK B1 RADFRAC
   IN-UNITS ENG
   PARAM NSTAGE=30
```

```
   COL-CONFIG CONDENSER=TOTAL
   RATESEP-ENAB CALC-MODE=EQUILIBRIUM
   FEEDS 1 8
   PRODUCTS 2 1 L / 3 30 L
   P-SPEC 1 0.9 <MPa>
   COL-SPECS D:F=0.5 MOLE-RR=9.
   REAC-STAGES 8 20 R-1
   HOLD-UP 1 29 MOLE-LHLDP=5. <mol> / 30 30  &
      MOLE-LHLDP=10. <mol>
   USERK-VECS NINT=5

EO-CONV-OPTI

SENSITIVITY S-2
   DEFINE XD BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
      ID1=METHANOL ID2=22
   TABULATE 2 "XD"
   VARY BLOCK-VAR BLOCK=B1 VARIABLE=MOLE-LHLDP SENTENCE=HOLD-UP  &
      ID1=1 LABEL="HOLDUP"
   RANGE LOWER="5" UPPER="6" NPOINT="10"

STREAM-REPOR MOLEFLOW

REACTIONS R-1 REAC-DIST
   IN-UNITS ENG
   REAC-DATA 1 KINETIC
   RATE-CON 1 PRE-EXP=4720. ACT-ENERGY=51700. <kJ/kmol>
   STOIC 1 METHANOL -2. / WATER 1. / DIMET-01 1.
   POWLAW-EXP 1 METHANOL 1.
```

User define kinetic subroutine fortran file

```
SUBROUTINE USRKNT      (N,    NCOMP,  NR,    NRL,    NRV,
   2                   T,    TLIQ,   TVAP,  P,      PHFRAC,
   3                   F,    X,      Y,     IDX,    NBOPST,
   4                   KDIAG, STOIC,  IHLBAS, HLDLIQ, TIMLIQ,
   5                   IHVBAS, HLDVAP, TIMVAP, NINT,  INT,
   6                   NREAL, REAL,   RATES, RATEL,  RATEV,
   7                   NINTB, INTB,   NREALB, REALB,  NIWORK,
   8                   IWORK, NWORK,  WORK)

INTEGER NRL(3),IDX(NCOMP),  NBOPST(6),
   +      INT(NINT),   INTB(NINTB),
   +      IWORK(NIWORK),N,    KDIAG, IHLBAS,
   +      IHVBAS,NREAL
    REAL*8 PHFRAC(3),   X(NCOMP,3),  Y(NCOMP),
   +     STOIC(NCOMP,NR),    RATES(NCOMP),
   +     RATEL(1),    RATEV(NRV),
   +     REALB(NREALB),WORK(NWORK), T,    TLIQ,
   +     TVAP, P,    F,    HLDLIQ,TIMLIQ

    REAL*8 HLDVAP,TIMVAP

    INTEGER IMISS
    REAL*8 REAL(NREAL), RMISS
    REAL*8 Cm, Cw, Rate, Kw, Ks

    Cm=13*X(2,3)
    Cw=13*X(1,3)
    Ks=4.72*EXP(-51700.0/8.314/T)
    Kw=EXP(-25.75+11138.0/T)
    RATE=HLDLIQ*ks*Cm*Cm/(Kw*Cw+Cm)

    RATES(3)=RATE
    RATES(1)=RATE
    RATES(2)=-RATE

    RETURN
    END
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
1	----	B1	2	B1	----
3	B1	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
B1	1	2 3

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS: B1

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL				
COMPONENTS (LBMOL/HR)				
WATER	0.00000	9.92080	9.92080	0.521697E-08
METHANOL	19.8416	0.211676E-05	-19.8416	-0.521698E-08
DIMET-01	0.00000	9.92080	9.92080	0.521697E-08
TOTAL BALANCE				
MOLE(LBMOL/HR)	19.8416	19.8416	0.00000	-0.340202E-14
MASS(LB/HR)	635.768	635.768		-0.411282E-14
ENTHALPY(BTU/HR)	-0.203534E+07	-0.202147E+07		-0.681285E-02

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
WATER	C	H2O	WATER
METHANOL	C	CH4O	METHANOL
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER

U-O-S BLOCK SECTION

```
BLOCK:  B1      MODEL: RADFRAC
------------------------------
 INLETS           - 1       STAGE   8
 OUTLETS          - 2       STAGE   1
                    3       STAGE  30
 PROPERTY OPTION SET:   NRTL     RENON (NRTL) / IDEAL GAS

                              ***  MASS AND ENERGY BALANCE  ***
                  IN        OUT      GENERATION   RELATIVE DIFF.
 TOTAL BALANCE
 MOLE(LBMOL/HR)       19.8416      19.8416      0.00000     -0.340202E-14
 MASS(LB/HR  )       635.768      635.768              -0.411282E-14
 ENTHALPY(BTU/HR  )  -0.203534E+07 -0.202147E+07            -0.681285E-02

            ***  CO2 EQUIVALENT SUMMARY ***
 FEED STREAMS CO2E          0.00000     LB/HR
 PRODUCT STREAMS CO2E       457.042     LB/HR
 NET STREAMS CO2E PRODUCTION  457.042     LB/HR
 UTILITIES CO2E PRODUCTION    0.00000     LB/HR
 TOTAL CO2E PRODUCTION       457.042     LB/HR

                                 **********************
                                 ****     INPUT DATA   ****
                                 **********************
 ****   INPUT PARAMETERS   ****

 NUMBER OF STAGES                                    30
 ALGORITHM OPTION                                    STANDARD
 INITIALIZATION OPTION                               STANDARD
 HYDRAULIC PARAMETER CALCULATIONS                    NO
 INSIDE LOOP CONVERGENCE METHOD                      NEWTON
 DESIGN SPECIFICATION METHOD                          NESTED
 MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS              25
 MAXIMUM NO. OF INSIDE LOOP ITERATIONS               10
 MAXIMUM NUMBER OF FLASH ITERATIONS                  30
 FLASH TOLERANCE                                     0.000100000
 OUTSIDE LOOP CONVERGENCE TOLERANCE                  0.000100000

 ****   COL-SPECS   ****

 MOLAR VAPOR DIST / TOTAL DIST                          0.0
 MOLAR REFLUX RATIO                                  9.00000
 DISTILLATE TO FEED RATIO                            0.50000

 **** REAC-STAGES SPECIFICATIONS ****

 STAGE  TO  STAGE         REACTIONS/CHEMISTRY ID
  8       20              R-1
```

**** RESIDENCE TIME SPECIFICATIONS ****

STAGE	TO STAGE	RESIDENCE TIME LIQUID PHASE	VAPOR PHASE
8	20	1.6667-02 HR	MISSING

***** REACTION PARAGRAPH R-1 *****

**** REACTION PARAMETERS ****

RXN NO.	TYPE	PHASE BASIS	CONC. F	TEMP APP TO EQUIL	CONVERSION
1	KINETIC	LIQUID	MOLAR		

** STOICHIOMETRIC COEFFICIENTS **

RXN NO.	WATER	METHANOL	DIMET-01
1	1.000	-2.000	1.000

** COEFFICIENTS IN GENERAL POWER LAW EXPRESSION **

RXN NO.	PRE-EXPONENTIAL FACTOR	ACTIVATION ENERGY BTU/LBMOL	TEMPERATURE EXPONENT
1	4720.0	22227.	0.0000

** COMPONENT EXPONENTS IN GENERAL POWER LAW EXPRESSION **

RXN NO.	WATER	METHANOL	DIMET-01
1	0.000	1.000	0.000

**** PROFILES ****

P-SPEC STAGE 1 PRES, PSIA 130.534

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	2	3
COMPONENT:		
WATER	0.0000	1.0000
METHANOL	.50022	.49978
DIMET-01	1.0000	.47414E-10

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	104.490
BOTTOM STAGE TEMPERATURE	F	347.805
TOP STAGE LIQUID FLOW	LBMOL/HR	89.2872
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	9.92080
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	48.2770
MOLAR REFLUX RATIO		9.00000
MOLAR BOILUP RATIO		4.86624
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-747,077.
REBOILER DUTY	BTU/HR	760,943.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.35800E-04	STAGE= 7	
BUBBLE POINT	0.13802E-03	STAGE= 20	
COMPONENT MASS BALANCE	0.14081E-06	STAGE= 22	COMP=DIMET-01
ENERGY BALANCE	0.81861E-04	STAGE= 21	

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE	PRESSURE	ENTHALPY BTU/LBMOL		HEAT DUTY
	F	PSIA	LIQUID	VAPOR	BTU/HR
1	104.49	130.53	-86241.	-78710.	-.74708+06
2	104.49	130.53	-86241.	-78710.	
7	106.12	130.53	-86591.	-78707.	
8	116.35	130.53	-88871.	-78695.	
9	116.22	130.53	-88890.	-78693.	
10	116.08	130.53	-88908.	-78691.	
29	347.81	130.53	-0.11752E+06	-0.10176E+06	
30	347.81	130.53	-0.11752E+06	-0.10176E+06	.76094+06

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	99.21	0.000				9.9208	
2	89.29	99.21					
7	85.13	98.63					
8	112.6	95.05	19.8416				
9	112.4	102.7					
10	112.2	102.5					
29	58.20	48.28					
30	9.921	48.28				9.9208	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	4570.	0.000				457.0418	
2	4113.	4570.					
7	3890.	4539.					
8	4876.	4347.	635.7678				
9	4866.	4697.					
10	4857.	4688.					
29	1048.	869.7					
30	178.7	869.7				178.7260	

**** MOLE-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.20551E-16	0.10673E-06	1.0000
2	0.24680E-14	0.92348E-06	1.0000
7	0.35113E-04	0.26454E-01	0.97351
8	0.29955E-02	0.19131	0.80570
9	0.58621E-02	0.18537	0.80877
10	0.86320E-02	0.17962	0.81175
29	1.0000	0.68801E-06	0.48416E-09
30	1.0000	0.10664E-06	0.47414E-10

**** MOLE-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.17113E-18	0.12335E-07	1.0000
2	0.20551E-16	0.10673E-06	1.0000
7	0.30174E-06	0.30935E-02	0.99691
8	0.31449E-04	0.23693E-01	0.97628
9	0.61534E-04	0.23003E-01	0.97694
10	0.90592E-04	0.22331E-01	0.97758
29	0.99999	0.52098E-05	0.58602E-08
30	1.0000	0.80748E-06	0.57391E-09

**** K-VALUES ****

STAGE	WATER	METHANOL	DIMET-01
1	0.83270E-02	0.11557	1.0000
2	0.83270E-02	0.11557	1.0000
7	0.85934E-02	0.11694	1.0241
8	0.10498E-01	0.12385	1.2117
9	0.10497E-01	0.12409	1.2079
10	0.10495E-01	0.12432	1.2043
29	1.0000	7.5723	12.104
30	1.0000	7.5723	12.104

**** RATES OF GENERATION ****

LBMOL/HR

STAGE	WATER	METHANOL	DIMET-01
1	0.000	0.000	0.000
2	0.000	0.000	0.000
7	0.000	0.000	0.000
8	0.3310	-.6620	0.3310
9	0.3185	-.6370	0.3185
10	0.3065	-.6131	0.3065
29	0.000	0.000	0.000
30	0.000	0.000	0.000

**** MASS-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.80364E-17	0.74234E-07	1.0000
2	0.96510E-15	0.64231E-06	1.0000
7	0.13843E-04	0.18549E-01	0.98144
8	0.12463E-02	0.14156	0.85719
9	0.24387E-02	0.13716	0.86040
10	0.35908E-02	0.13290	0.86351
29	1.0000	0.12237E-05	0.12381E-08

**** MASS-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
30	1.0000	0.18966E-06	0.12125E-09

**** MASS-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.66919E-19	0.85795E-08	1.0000
2	0.80364E-17	0.74234E-07	1.0000
7	0.11811E-06	0.21536E-02	0.99785
8	0.12388E-04	0.16599E-01	0.98339
9	0.24233E-04	0.16112E-01	0.98386
10	0.35671E-04	0.15639E-01	0.98433
29	0.99999	0.92661E-05	0.14986E-07
30	1.0000	0.14362E-05	0.14676E-08

STREAM SECTION

1 2 3

STREAM ID	1	2	3
FROM :	----	B1	B1
TO :	B1	----	----

SUBSTREAM: MIXED

PHASE:	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR			
WATER	0.0	2.0388-16	9.9208
METHANOL	19.8416	1.0589-06	1.0579-06
DIMET-01	0.0	9.9208	4.7039-10
TOTAL FLOW:			
LBMOL/HR	19.8416	9.9208	9.9208
LB/HR	635.7678	457.0418	178.7260
CUFT/HR	12.8408	11.6390	3.4361
STATE VARIABLES:			
TEMP F	76.7300	104.4905	347.8054
PRES PSIA	130.5340	130.5340	130.5340
VFRAC	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0
ENTHALPY:			
BTU/LBMOL	-1.0258+05	-8.6241+04	-1.1752+05
BTU/LB	-3201.3819	-1871.9906	-6523.3430
BTU/HR	-2.0353+06	-8.5558+05	-1.1659+06
ENTROPY:			
BTU/LBMOL-R	-57.5409	-74.0066	-31.1306
BTU/LB-R	-1.7958	-1.6064	-1.7280
DENSITY:			
LBMOL/CUFT	1.5452	0.8524	2.8872
LB/CUFT	49.5116	39.2681	52.0139
AVG MW	32.0422	46.0690	18.0153

PROBLEM STATUS SECTION

BLOCK STATUS

```
**********************************************************************
*                                                                    *
* Calculations were completed normally                               *
*                                                                    *
* All Unit Operation blocks were completed normally                  *
*                                                                    *
* All streams were flashed normally                                  *
*                                                                    *
**********************************************************************
```

Appendix C

Aspen files: DME CD process of Langmuir-Hinshelwood model

```
DYNAMICS
   DYNAMICS RESULTS=ON

IN-UNITS SI MOLE-FLOW='mol/sec' MOLES=mol

DEF-STREAMS CONVEN ALL

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS MASS-BAL-CHE=YES OLD-DATABANK=YES

DATABANKS PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      NOASPENPCD

PROP-SOURCES PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
   WATER H2O /
   METHANOL CH4O /
   DIMET-01 C2H6O-1

FLOWSHEET
   BLOCK B1 IN=1 OUT=2 3

PROPERTIES NRTL
   PROPERTIES IDEAL / NRTL-SAC

PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL WATER METHANOL 2.732200000 -1111.083651 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL WATER -.6930000000 311.3767775 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL DIMET-01 0.0 1175.411331 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374
   BPVAL DIMET-01 METHANOL 0.0 -34.08695973 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374

STREAM 1
   IN-UNITS ENG
   SUBSTREAM MIXED TEMP=298. <K> PRES=0.9 <MPa>  &
      MOLE-FLOW=2.5 <mol/sec>
   MOLE-FRAC METHANOL 1.
```

```
BLOCK B1 RADFRAC
   IN-UNITS ENG
   PARAM NSTAGE=30
   COL-CONFIG CONDENSER=TOTAL
   RATESEP-ENAB CALC-MODE=EQUILIBRIUM
   FEEDS 1 8
   PRODUCTS 2 1 L / 3 30 L
   P-SPEC 1 0.9 <MPa>
   COL-SPECS D:F=0.5 MOLE-RR=9.
   REAC-STAGES 8 20 R-1
   HOLD-UP 8 20 MASS-LHLDP=9.23 <kg>
   USERK-VECS NINT=5

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW

REACTIONS R-1 REAC-DIST
   IN-UNITS ENG
   PARAM SUBROUTINE=USRKNT
   REAC-DATA 1 KINETIC
   STOIC 1 METHANOL -2. / WATER 1. / DIMET-01 1.
```

User define kinetic subroutine fortran file

```
SUBROUTINE USRKNT      (N,    NCOMP,  NR,    NRL,    NRV,
   2                   T,    TLIQ,   TVAP,  P,      PHFRAC,
   3                   F,    X,      Y,     IDX,    NBOPST,
   4                   KDIAG, STOIC,  IHLBAS, HLDLIQ, TIMLIQ,
   5                   IHVBAS, HLDVAP, TIMVAP, NINT,  INT,
   6                   NREAL, REAL,   RATES, RATEL,  RATEV,
   7                   NINTB, INTB,   NREALB, REALB,  NIWORK,
   8                   IWORK, NWORK,  WORK)

    INTEGER NRL(3),IDX(NCOMP),  NBOPST(6),
   +      INT(NINT),   INTB(NINTB),
   +      IWORK(NIWORK),N,    KDIAG, IHLBAS,
   +      IHVBAS,NREAL
    REAL*8 PHFRAC(3),   X(NCOMP,3),  Y(NCOMP),
   +     STOIC(NCOMP,NR),    RATES(NCOMP),
   +     RATEL(1),    RATEV(NRV),
   +     REALB(NREALB),WORK(NWORK), T,    TLIQ,
   +     TVAP, P,    F,    HLDLIQ,TIMLIQ

    REAL*8 HLDVAP,TIMVAP
    INTEGER IMISS
    REAL*8 REAL(NREAL), RMISS
    REAL*8 Cm, Cw, Rate, Kw, Ks
    Cm=13*X(2,3)
    Cw=13*X(1,3)
    Ks=61200000*EXP(-98000.0/8.314/T)
    Kw=EXP(-6.46+2964.0/T)
    RATE=HLDLIQ*ks*Cm*Cm/(Kw*Cw+Cm)*(Kw*Cw+Cm)
    RATES(3)=RATE
    RATES(1)=RATE
    RATES(2)=-RATE

    RETURN
    END
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
1	----	B1	2	B1	----
3	B1	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
B1	1	2 3

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
B1

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (MOL/SEC)				
WATER	0.00000	1.04356	1.04356	0.172470E-09
METHANOL	2.50000	0.412876	-2.08712	-0.143985E-09
DIMET-01	0.00000	1.04356	1.04356	0.172468E-09
TOTAL BALANCE				
MOLE(MOL/SEC)	2.50000	2.50000	0.00000	0.106581E-14
MASS(KG/SEC)	0.801054E-01	0.801054E-01		0.692976E-15
ENTHALPY(WATT)	-596498.	-590834.		-0.949475E-02

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
WATER	C	H2O	WATER
METHANOL	C	CH4O	METHANOL
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER

U-O-S BLOCK SECTION

BLOCK: B1 MODEL: RADFRAC

INLETS - 1 STAGE 8
OUTLETS - 2 STAGE 1
3 STAGE 30
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(MOL/SEC)	2.50000	2.50000	0.00000	0.106581E-14
MASS(KG/SEC)	0.801054E-01	0.801054E-01		0.692976E-15
ENTHALPY(WATT)	-596498.	-590834.		-0.949475E-02

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E 0.00000 KG/SEC
PRODUCT STREAMS CO2E 0.480759E-01 KG/SEC
NET STREAMS CO2E PRODUCTION 0.480759E-01 KG/SEC
UTILITIES CO2E PRODUCTION 0.00000 KG/SEC
TOTAL CO2E PRODUCTION 0.480759E-01 KG/SEC

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	30
ALGORITHM OPTION	STANDARD
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	9.00000
DISTILLATE TO FEED RATIO	0.50000

**** REAC-STAGES SPECIFICATIONS ****

STAGE	TO STAGE	REACTIONS/CHEMISTRY ID
8	20	R-1

**** HOLD-UP SPECIFICATIONS ****

STAGE	TO STAGE	LIQUID HOLDUP	VAPOR HOLDUP
8	20	9.2300 KG	MISSING

***** REACTION PARAGRAPH R-1 *****

**** REACTION PARAMETERS ****

RXN NO.	TYPE	PHASE BASIS	CONC. K	TEMP APP TO EQUIL	CONVERSION
1	KINETIC	LIQUID	MOLAR		

** STOICHIOMETRIC COEFFICIENTS **

RXN NO.	WATER	METHANOL	DIMET-01
1	1.000	-2.000	1.000

**** PROFILES ****

P-SPEC STAGE 1 PRES, N/SQM 900,000.

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	2	3
COMPONENT:		
WATER	.55806E-04	.99994
METHANOL	.49986	.50014
DIMET-01	1.0000	.36813E-14

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	K	319.019
BOTTOM STAGE TEMPERATURE	K	427.265
TOP STAGE LIQUID FLOW	MOL/SEC	11.2500
BOTTOM STAGE LIQUID FLOW	MOL/SEC	1.25000
TOP STAGE VAPOR FLOW	MOL/SEC	0.0
BOILUP VAPOR FLOW	MOL/SEC	8.11669
MOLAR REFLUX RATIO		9.00000
MOLAR BOILUP RATIO		6.49336
CONDENSER DUTY (W/O SUBCOOL)	WATT	-277,084.
REBOILER DUTY	WATT	282,748.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.15517E-05	STAGE= 1
BUBBLE POINT	0.26450E-03	STAGE= 2
COMPONENT MASS BALANCE	0.33537E-06	STAGE= 1 COMP=WATER
ENERGY BALANCE	0.22044E-04	STAGE= 3

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE K	PRESSURE N/SQM	ENTHALPY J/KMOL LIQUID	VAPOR	HEAT DUTY WATT
1	319.02	0.90000E+06	-0.20567E+09	-0.18305E+09	-.27708+06
2	349.94	0.90000E+06	-0.22861E+09	-0.18351E+09	
3	397.31	0.90000E+06	-0.22646E+09	-0.19216E+09	
7	401.68	0.90000E+06	-0.22672E+09	-0.19408E+09	
8	401.85	0.90000E+06	-0.22728E+09	-0.19430E+09	
9	402.81	0.90000E+06	-0.22796E+09	-0.19492E+09	
29	416.71	0.90000E+06	-0.25336E+09	-0.20781E+09	
30	427.26	0.90000E+06	-0.26700E+09	-0.21643E+09	.28275+06

STAGE	FLOW RATE MOL/SEC		FEED RATE MOL/SEC			PRODUCT RATE MOL/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	12.50	0.000				1.2500	
2	7.139	12.50					
3	8.017	8.389					
7	8.110	9.376					
8	11.52	9.360	2.5000				
9	11.43	10.27					
29	9.367	8.635					
30	1.250	8.117				1.2500	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/SEC		FEED RATE KG/SEC			PRODUCT RATE KG/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5469	0.000				.54690-01	
2	0.2390	0.5469					
3	0.2576	0.2936					
7	0.2586	0.3146					
8	0.3656	0.3133	.80105-01				
9	0.3602	0.3402					
29	0.2275	0.2408					
30	0.2542E-01	0.2021				.25416-01	

**** MOLE-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.46589E-04	0.16510	0.83485
2	0.81418E-03	0.89644	0.10275
3	0.16199E-02	0.99032	0.80552E-02
7	0.15150E-01	0.98063	0.42238E-02
8	0.26508E-01	0.96911	0.43776E-02
9	0.41406E-01	0.95477	0.38286E-02
29	0.55264	0.44736	0.23733E-13
30	0.83480	0.16520	0.30733E-14

**** MOLE-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.47110E-06	0.20250E-01	0.97975
2	0.46590E-04	0.16510	0.83485
3	0.69981E-03	0.78747	0.21183
7	0.75243E-02	0.87759	0.11489
8	0.13133E-01	0.87172	0.11515
9	0.20949E-01	0.88134	0.97711E-01
29	0.29612	0.70388	0.23532E-12
30	0.50918	0.49082	0.26914E-13

**** K-VALUES ****

STAGE	WATER	METHANOL	DIMET-01
1	0.10112E-01	0.12265	1.1736
2	0.57233E-01	0.18417	8.1280
3	0.43200	0.79516	26.297
7	0.49667	0.89493	27.200
8	0.49543	0.89950	26.304
9	0.50595	0.92310	25.521
29	0.53584	1.5734	9.9155
30	0.60995	2.9711	8.7573

**** RATES OF GENERATION ****

MOL/SEC

STAGE	WATER	METHANOL	DIMET-01
1	0.000	0.000	0.000
2	0.000	0.000	0.000
3	0.000	0.000	0.000
7	0.000	0.000	0.000
8	0.9029E-01	-.1806	0.9029E-01
9	0.9023E-01	-.1805	0.9023E-01
29	0.000	0.000	0.000
30	0.000	0.000	0.000

**** MASS-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.19184E-04	0.12092	0.87907
2	0.43821E-03	0.85815	0.14141
3	0.90822E-03	0.98754	0.11549E-01
7	0.85586E-02	0.98534	0.61020E-02
8	0.15049E-01	0.97860	0.63555E-02
9	0.23670E-01	0.97073	0.55967E-02
29	0.40987	0.59013	0.45011E-13
30	0.73966	0.26034	0.69635E-14

**** MASS-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.18537E-06	0.14172E-01	0.98583
2	0.19184E-04	0.12092	0.87907
3	0.36017E-03	0.72084	0.27880
7	0.40406E-02	0.83819	0.15776
8	0.70680E-02	0.83445	0.15848
9	0.11396E-01	0.85269	0.13592
29	0.19129	0.80871	0.38873E-12
30	0.36840	0.63160	0.49796E-13

STREAM SECTION

1 2 3

STREAM ID	1	2	3
FROM :	----	B1	B1
TO :	B1	----	----

SUBSTREAM: MIXED			
PHASE:	LIQUID	LIQUID	LIQUID
COMPONENTS: MOL/SEC			
WATER	0.0	5.8237-05	1.0435
METHANOL	2.5000	0.2064	0.2065
DIMET-01	0.0	1.0436	3.8417-15
TOTAL FLOW:			
MOL/SEC	2.5000	1.2500	1.2500
KG/SEC	8.0105-02	5.4690-02	2.5416-02
CUM/SEC	1.0100-04	8.5112-05	3.2510-05
STATE VARIABLES:			
TEMP K	298.0000	319.0188	427.2647
PRES N/SQM	9.0000+05	9.0000+05	9.0000+05
VFRAC	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0
ENTHALPY:			
J/KMOL	-2.3860+08	-2.0567+08	-2.6700+08
J/KG	-7.4464+06	-4.7009+06	-1.3131+07
WATT	-5.9650+05	-2.5709+05	-3.3374+05
ENTROPY:			
J/KMOL-K	-2.4091+05	-2.9245+05	-1.4359+05
J/KG-K	-7518.5980	-6684.2943	-7061.9876
DENSITY:			
KMOL/CUM	24.7517	14.6865	38.4496
KG/CUM	793.0991	642.5602	781.7754
AVG MW	32.0422	43.7518	20.3325

PROBLEM STATUS SECTION

BLOCK STATUS

```
**************************************************************************
*                                                                        *
* Calculations were completed normally                                   *
*                                                                        *
* All Unit Operation blocks were completed normally                      *
*                                                                        *
* All streams were flashed normally                                      *
*                                                                        *
**************************************************************************
```

Appendix D

Aspen files: CD process Parameter Analysis

```
DYNAMICS
   DYNAMICS RESULTS=ON

IN-UNITS SI MOLE-FLOW='mol/sec' MOLES=mol

DEF-STREAMS CONVEN ALL

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS MASS-BAL-CHE=YES OLD-DATABANK=YES

DATABANKS PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      NOASPENPCD

PROP-SOURCES PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
   WATER H2O /
   METHANOL CH4O /
   DIMET-01 C2H6O-1

FLOWSHEET
   BLOCK B1 IN=1 OUT=2 3

PROPERTIES NRTL
   PROPERTIES IDEAL / NRTL-SAC

PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL WATER METHANOL 2.732200000 -1111.083651 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL WATER -.6930000000 311.3767775 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL DIMET-01 0.0 1175.411331 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374
   BPVAL DIMET-01 METHANOL 0.0 -34.08695973 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374

STREAM 1
   IN-UNITS ENG
   SUBSTREAM MIXED TEMP=298. <K> PRES=0.9 <MPa>  &
      MOLE-FLOW=2.5 <mol/sec>
   MOLE-FRAC METHANOL 1.
```

```
BLOCK B1 RADFRAC
   IN-UNITS ENG
   PARAM NSTAGE=25
   COL-CONFIG CONDENSER=TOTAL
   RATESEP-ENAB CALC-MODE=EQUILIBRIUM
   FEEDS 1 8
   PRODUCTS 2 1 L / 3 25 L
   P-SPEC 1 0.9 <MPa>
   COL-SPECS D:F=0.5 MOLE-RR=8.
   REAC-STAGES 8 20 R-1
   HOLD-UP 8 20 MASS-LHLDP=15. <kg>
   USERK-VECS NINT=5

EO-CONV-OPTI

SENSITIVITY S-3
   DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   TABULATE 1 "DMEVP"
   TABULATE 2 "DMELQ"
   VARY BLOCK-VAR BLOCK=B1 VARIABLE=NSTAGE SENTENCE=PARAM
   RANGE LOWER="10" UPPER="40" NPOINT="7"

SENSITIVITY S-4
   DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   TABULATE 1 "DMEVP"
   TABULATE 2 "DMELQ"
   VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE SENTENCE=FEEDS ID1=1
   RANGE LOWER="6" UPPER="40" INCR="2"

SENSITIVITY S-5
   DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   TABULATE 1 "DMEVP"
   TABULATE 2 "DMELQ"
   VARY BLOCK-VAR BLOCK=B1 VARIABLE=MOLE-RR SENTENCE=COL-SPECS
   RANGE LOWER="2" UPPER="10" INCR="1"

SENSITIVITY S-6
   DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
      ID1=DIMET-01 ID2=1
   TABULATE 1 "DMEVP"
```

```
  TABULATE 2 "DMELQ"
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=MASS-LHLDP SENTENCE=HOLD-UP  &
    ID1=8
  RANGE LOWER="5" UPPER="20" INCR="2.5"

SENSITIVITY S-7
  DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  TABULATE 1 "DMEVP"
  TABULATE 2 "DMELQ"
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE1 SENTENCE=REAC-STAGES  &
    ID1=8
  RANGE LOWER="6" UPPER="15" INCR="1"

SENSITIVITY S-8
  DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  TABULATE 1 "DMEVP"
  TABULATE 2 "DMELQ"
  VARY STREAM-VAR STREAM=1 SUBSTREAM=MIXED VARIABLE=MOLE-FLOW
  RANGE LOWER="1" UPPER="10" INCR="0.5"

SENSITIVITY S-9
  DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  TABULATE 1 "DMEVP"
  TABULATE 2 "DMELQ"
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE2 SENTENCE=REAC-STAGES  &
    ID1=8
  RANGE LOWER="10" UPPER="25" INCR="1"

SENSITIVITY S-10
  PARAM CASES=YES
  DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE TEMP16 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
    SENTENCE=PROFILE ID1=16
  DEFINE TEMP18 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
    SENTENCE=PROFILE ID1=18
  DEFINE TEMP20 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
    SENTENCE=PROFILE ID1=20
  DEFINE TEMP22 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
    SENTENCE=PROFILE ID1=22
  DEFINE TEMP24 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
```

```
    SENTENCE=PROFILE ID1=24
  TABULATE 1 "DMEVP"
  TABULATE 2 "DMELQ"
  TABULATE 3 "TEMP16"
  TABULATE 4 "TEMP18"
  TABULATE 5 "TEMP20"
  TABULATE 6 "TEMP22"
  TABULATE 7 "TEMP24"
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE1 SENTENCE=REAC-STAGES  &
    ID1=8
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE2 SENTENCE=REAC-STAGES  &
    ID1=8
  VARY BLOCK-VAR BLOCK=B1 VARIABLE=STAGE SENTENCE=FEEDS ID1=1
  CASES 1 DESCRIP="4-16" VALUES= 4. 16. 4.
  CASES 2 DESCRIP="6-18" VALUES= 6. 18. 6.
  CASES 3 DESCRIP="8-20" VALUES= 8. 20. 8.
  CASES 4 DESCRIP="10-22" VALUES= 10. 22. 10.
  CASES 5 DESCRIP="12-24" VALUES= 12. 24. 12.

SENSITIVITY S-11
  PARAM CASES=YES
  DEFINE DMEVP BLOCK-VAR BLOCK=B1 VARIABLE=Y SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE DMELQ BLOCK-VAR BLOCK=B1 VARIABLE=X SENTENCE=COMPS  &
    ID1=DIMET-01 ID2=1
  DEFINE TEMP20 BLOCK-VAR BLOCK=B1 VARIABLE=TEMP  &
    SENTENCE=PROFILE ID1=20
  TABULATE 1 "DMEVP"
  TABULATE 2 "DMELQ"
  TABULATE 3 "TEMP20"
  VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED COMPONENT=METHANOL
  VARY MOLE-FLOW STREAM=1 SUBSTREAM=MIXED COMPONENT=WATER
  CASES 1 DESCRIP="100%" VALUES= 2.5 0.
  CASES 2 DESCRIP="95%" VALUES= 2.375 0.125
  CASES 3 DESCRIP="90%" VALUES= 2.25 0.25
  CASES 4 DESCRIP="85%" VALUES= 2.125 0.375
  CASES 5 DESCRIP="80%" VALUES= 2. 0.5

STREAM-REPOR MOLEFLOW MOLEFRAC

REACTIONS R-1 REAC-DIST
  IN-UNITS ENG
  PARAM SUBROUTINE=USRKNT
  REAC-DATA 1 KINETIC
  STOIC 1 METHANOL -2. / WATER 1. / DIMET-01 1.
```

User define kinetic subroutine fortran file

```
SUBROUTINE USRKNT      (N,    NCOMP,  NR,    NRL,    NRV,
   2                   T,    TLIQ,   TVAP,  P,      PHFRAC,
   3                   F,    X,      Y,     IDX,    NBOPST,
   4                   KDIAG, STOIC,  IHLBAS, HLDLIQ, TIMLIQ,
   5                   IHVBAS, HLDVAP, TIMVAP, NINT,  INT,
   6                   NREAL, REAL,   RATES, RATEL,  RATEV,
   7                   NINTB, INTB,   NREALB, REALB,  NIWORK,
   8                   IWORK, NWORK,  WORK)

    INTEGER NRL(3),IDX(NCOMP),  NBOPST(6),
   +      INT(NINT),   INTB(NINTB),
   +      IWORK(NIWORK),N,    KDIAG, IHLBAS,
   +      IHVBAS,NREAL
    REAL*8 PHFRAC(3),   X(NCOMP,3),  Y(NCOMP),
   +     STOIC(NCOMP,NR),    RATES(NCOMP),
   +     RATEL(1),    RATEV(NRV),
   +     REALB(NREALB),WORK(NWORK), T,    TLIQ,
   +     TVAP, P,    F,    HLDLIQ,TIMLIQ

    REAL*8 HLDVAP,TIMVAP
    INTEGER IMISS
    REAL*8 REAL(NREAL), RMISS
    REAL*8 Cm, Cw, Rate, Kw, Ks
    Cm=13*X(2,3)
    Cw=13*X(1,3)
    Ks=61200000*EXP(-98000.0/8.314/T)
    Kw=EXP(-6.46+2964.0/T)
    RATE=HLDLIQ*ks*Cm*Cm/(Kw*Cw+Cm)*(Kw*Cw+Cm)
    RATES(3)=RATE
    RATES(1)=RATE
    RATES(2)=-RATE

    RETURN
    END
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
1	----	B1	2	B1	----
3	B1	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
B1	1	2 3

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

```
 S-3
 | S-4
 | | S-5
 | | | S-6
 | | | | S-7
 | | | | | S-8
 | | | | | | S-9
 | | | | | | | S-10
 | | | | | | | | S-11 B1
 | | | | | | | | (RETURN S-11)
 | | | | | | | (RETURN S-10)
 | | | | | | (RETURN S-9)
 | | | | | (RETURN S-8)
 | | | | (RETURN S-7)
 | | | (RETURN S-6)
 | | (RETURN S-5)
 | (RETURN S-4)
 (RETURN S-3)
```

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS				
(MOL/SEC)				
WATER	0.00000	1.24337	1.24337	-0.393160E-10
METHANOL	2.50000	0.132658E-01	-2.48673	0.391088E-10
DIMET-01	0.00000	1.24337	1.24337	-0.393148E-10
TOTAL BALANCE				
MOLE(MOL/SEC)	2.50000	2.50000	0.00000	0.195399E-14
MASS(KG/SEC)	0.801054E-01	0.801054E-01		0.225217E-14
ENTHALPY(WATT)	-596498.	-592474.		-0.674604E-02

SENSITIVITY BLOCK SECTION

SENSITIVITY BLOCK: S-3

SAMPLED VARIABLES:
DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:
VARY 1: SENTENCE=PARAM VARIABLE=NSTAGE IN UOS BLOCK B1
LOWER LIMIT = 10.0000
UPPER LIMIT = 40.0000
POINTS = 7

TABULATED VARIABLES:
COLUMN 2: DMEVP
COLUMN 3: DMELQ

VARY 1 B1 PARAM NSTAGE	DMEVP	DMELQ
10.0000	0.9132	0.2923
15.0000	0.9594	0.6766
20.0000	0.9899	0.9159
25.0000	0.9994	0.9947
e 30.0000	0.9994	0.9947
e 35.0000	0.9994	0.9947
e 40.0000	0.9994	0.9947
25.0000	0.9994	0.9947

e ERRORS OCCURRED FOR VALUES IN THIS ROW.
SEE THE HISTORY FILE FOR DETAILS.

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994694	

SENSITIVITY BLOCK: S-4

SAMPLED VARIABLES:

DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:

SENSITIVITY BLOCK SECTION

SENSITIVITY BLOCK: S-4 (CONTINUED)

VARY 1: SENTENCE=FEEDS VARIABLE=STAGE ID1=1 IN UOS BLOCK B1

LOWER LIMIT = 6.0000

UPPER LIMIT = 40.0000

INCREMENT = 2.0000

TABULATED VARIABLES:

COLUMN 2: DMEVP

COLUMN 3: DMELQ

VARY 1 B1 1 FEEDS STAGE	DMEVP	DMELQ
6.0000	0.9995	0.9959
8.0000	0.9994	0.9947
10.0000	0.9986	0.9882
12.0000	0.9969	0.9736
14.0000	0.9943	0.9520
16.0000	0.9910	0.9243
18.0000	0.9868	0.8904
20.0000	0.9815	0.8487
22.0000	0.9766	0.8103
24.0000	0.9744	0.7933
26.0000	0.9732	0.7835
28.0000	0.9732	0.7835
30.0000	0.9732	0.7835
32.0000	0.9732	0.7835
34.0000	0.9732	0.7835
36.0000	0.9732	0.7835
38.0000	0.9732	0.7835
40.0000	0.9732	0.7835
8.0000	0.9994	0.9947

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994694	

SENSITIVITY BLOCK: S-5

SAMPLED VARIABLES:

DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:

VARY 1: SENTENCE=COL-SPECS VARIABLE=MOLE-RR IN UOS BLOCK B1

LOWER LIMIT = 2.0000

UPPER LIMIT = 10.0000

INCREMENT = 1.0000

TABULATED VARIABLES:

COLUMN 2: DMEVP

COLUMN 3: DMELQ

VARY 1 B1 COL-SPEC MOLE-RR	DMEVP	DMELQ
2.0000	0.9711	0.7676
3.0000	0.9790	0.8286
4.0000	0.9851	0.8767
5.0000	0.9899	0.9154
6.0000	0.9938	0.9476
7.0000	0.9970	0.9746
8.0000	0.9994	0.9947
9.0000	1.0000	0.9996
10.0000	1.0000	0.9999
8.0000	0.9994	0.9947

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994693	

SENSITIVITY BLOCK: S-6

SAMPLED VARIABLES:
DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:
VARY 1: SENTENCE=HOLD-UP VARIABLE=MASS-LHLDP ID1=8 IN UOS BLOCK B1
LOWER LIMIT = 5.0000 KG
UPPER LIMIT = 20.0000 KG
INCREMENT = 2.5000

TABULATED VARIABLES:
COLUMN 2: DMEVP
COLUMN 3: DMELQ

VARY 1 B1 8 HOLD-UP MASS-LHL KG	DMEVP	DMELQ
5.0000	0.9442	0.5550
7.5000	0.9654	0.7232
10.0000	0.9813	0.8467
12.5000	0.9923	0.9349
15.0000	0.9994	0.9947
17.5000	1.0000	1.0000
20.0000	1.0000	1.0000
15.0000	0.9994	0.9947

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994693	

SENSITIVITY BLOCK: S-7

SAMPLED VARIABLES:
DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:
VARY 1: SENTENCE=REAC-STAGES VARIABLE=STAGE1 ID1=8 IN UOS BLOCK B1
LOWER LIMIT = 6.0000
UPPER LIMIT = 15.0000
INCREMENT = 1.0000

TABULATED VARIABLES:
COLUMN 2: DMEVP
COLUMN 3: DMELQ

VARY 1 B1 8 REAC-STA STAGE1	DMEVP	DMELQ
6.0000	0.9994	0.9947
7.0000	0.9994	0.9947
8.0000	0.9994	0.9947
9.0000	0.9965	0.9700
10.0000	0.9924	0.9356
11.0000	0.9874	0.8955
12.0000	0.9815	0.8487
13.0000	0.9746	0.7944
14.0000	0.9665	0.7325
15.0000	0.9575	0.6624
8.0000	0.9994	0.9947

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994693	

SENSITIVITY BLOCK: S-8

SAMPLED VARIABLES:
DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:
VARY 1: TOTAL MOLEFLOW IN STREAM 1 SUBSTREAM MIXED
LOWER LIMIT = 1.0000 MOL/SEC
UPPER LIMIT = 10.0000 MOL/SEC
INCREMENT = 0.5000

TABULATED VARIABLES:
COLUMN 2: DMEVP
COLUMN 3: DMELQ

VARY 1	DMEVP	DMELQ
1 MIXED TOTAL MOLEFLOW MOL/SEC		
e 1.0000	1.0000	1.0000
1.5000	1.0000	1.0000
2.0000	1.0000	1.0000
2.5000	0.9994	0.9947
3.0000	0.9923	0.9349
3.5000	0.9849	0.8751
4.0000	0.9778	0.8194
4.5000	0.9712	0.7688
5.0000	0.9654	0.7232
5.5000	0.9601	0.6823
6.0000	0.9554	0.6455
6.5000	0.9513	0.6124
7.0000	0.9475	0.5823
7.5000	0.9442	0.5550
8.0000	0.9413	0.5301
8.5000	0.9386	0.5073
9.0000	0.9362	0.4863
9.5000	0.9340	0.4670
10.0000	0.9320	0.4491
2.5000	0.9994	0.9947

e ERRORS OCCURRED FOR VALUES IN THIS ROW.
SEE THE HISTORY FILE FOR DETAILS.

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994695	

SENSITIVITY BLOCK: S-9

SAMPLED VARIABLES:
DMEVP : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
DMELQ : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1

VARIED VARIABLES:
VARY 1: SENTENCE=REAC-STAGES VARIABLE=STAGE2 ID1=8 IN UOS BLOCK B1
LOWER LIMIT = 10.0000
UPPER LIMIT = 25.0000
INCREMENT = 1.0000

TABULATED VARIABLES:
COLUMN 2: DMEVP
COLUMN 3: DMELQ

VARY 1 B1 8 REAC-STA STAGE2	DMEVP	DMELQ
10.0000	0.9264	0.4001
11.0000	0.9377	0.4996
12.0000	0.9482	0.5877
13.0000	0.9580	0.6661
14.0000	0.9670	0.7356
15.0000	0.9749	0.7969
16.0000	0.9818	0.8507
17.0000	0.9876	0.8970
18.0000	0.9925	0.9366
19.0000	0.9965	0.9705
20.0000	0.9994	0.9947
21.0000	0.9994	0.9947
22.0000	0.9994	0.9947
23.0000	0.9994	0.9947
24.0000	0.9994	0.9947

```
!------------+------------+------------!
!   25.0000 !    0.9994 !    0.9947 !
!   20.0000 !    0.9994 !    0.9947 !
----------------------------------------

 VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
  VARIABLE        VALUE       UNITS
  --------        -----       -----
  DMEVP         0.999385
  DMELQ         0.994694

SENSITIVITY BLOCK:  S-10
------------------------

 SAMPLED VARIABLES:
  DMEVP   : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
  DMELQ   : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
  TEMP16  : SENTENCE=PROFILE VARIABLE=TEMP ID1=16 IN UOS BLOCK B1
  TEMP18  : SENTENCE=PROFILE VARIABLE=TEMP ID1=18 IN UOS BLOCK B1
  TEMP20  : SENTENCE=PROFILE VARIABLE=TEMP ID1=20 IN UOS BLOCK B1
  TEMP22  : SENTENCE=PROFILE VARIABLE=TEMP ID1=22 IN UOS BLOCK B1
  TEMP24  : SENTENCE=PROFILE VARIABLE=TEMP ID1=24 IN UOS BLOCK B1

 VARIED VARIABLES:
  VARY   1: SENTENCE=REAC-STAGES VARIABLE=STAGE1 ID1=8 IN UOS BLOCK B1
  VARY   2: SENTENCE=REAC-STAGES VARIABLE=STAGE2 ID1=8 IN UOS BLOCK B1
  VARY   3: SENTENCE=FEEDS VARIABLE=STAGE ID1=1 IN UOS BLOCK B1

 TABULATED VARIABLES:
  COLUMN   4: DMEVP
  COLUMN   5: DMELQ
  COLUMN   6: TEMP16
  COLUMN   7: TEMP18
  COLUMN   8: TEMP20
  COLUMN   9: TEMP22
  COLUMN  10: TEMP24

 CASE INFORMATION:
  CASE   1: "4-16"
    VARY   1: 4.0000       VARY   2: 16.0000       VARY   3: 4.0000      CASE   2: "6-18"
    VARY   1: 6.0000       VARY   2: 18.0000       VARY   3: 6.0000      CASE   3: "8-20"
    VARY   1: 8.0000       VARY   2: 20.0000       VARY   3: 8.0000      CASE   4: "10-22"
    VARY   1: 10.0000       VARY   2: 22.0000       VARY   3: 10.0000      CASE   5: "12-24"
    VARY   1: 12.0000       VARY   2: 24.0000       VARY   3: 12.0000
```

```
-------------------------------------------------------------------------------
! VARY  1 ! VARY  2 ! VARY  3 ! DMEVP   ! DMELQ   ! TEMP16  !
! B1     ! B1     ! B1     !       !       !       !
! 8      ! 8      ! 1      !       !       !       !
! REAC-STA ! REAC-STA ! FEEDS   !       !       !       !
! STAGE1   ! STAGE2   ! STAGE   !       !       !       !
!        !        !        !       !       ! K     !
!        !        !        !       !       !       !
!============!============!============!============!============!============!
!   4.0000 !   16.0000 !   4.0000 !   0.9820 !   0.8528 !  409.1536 !
!   6.0000 !   18.0000 !   6.0000 !   0.9927 !   0.9388 !  408.3210 !
!   8.0000 !   20.0000 !   8.0000 !   0.9994 !   0.9947 !  407.3425 !
!  10.0000 !   22.0000 !  10.0000 !   0.9921 !   0.9335 !  406.4697 !
!  12.0000 !   24.0000 !  12.0000 !   0.9812 !   0.8465 !  405.6870 !
!------------+------------+------------+------------+------------+------------!
!   8.0000 !   20.0000 !   8.0000 !   0.9994 !   0.9947 !  407.3425 !
-------------------------------------------------------------------------------


-------------------------------------------------------------------------------
! VARY  1 ! VARY  2 ! VARY  3 ! TEMP18  ! TEMP20  ! TEMP22  !
! B1     ! B1     ! B1     !       !       !       !
! 8      ! 8      ! 1      !       !       !       !
! REAC-STA ! REAC-STA ! FEEDS   !       !       !       !
! STAGE1   ! STAGE2   ! STAGE   !       !       !       !
!        !        !        ! K     ! K     ! K     !
!        !        !        !       !       !       !
!============!============!============!============!============!============!
!   4.0000 !   16.0000 !   4.0000 !  409.7582 !  410.0090 !  411.1623 !
!   6.0000 !   18.0000 !   6.0000 !  410.0585 !  410.9569 !  412.6834 !
!   8.0000 !   20.0000 !   8.0000 !  409.3877 !  411.9869 !  418.2494 !
!  10.0000 !   22.0000 !  10.0000 !  408.3922 !  410.3558 !  412.5414 !
!  12.0000 !   24.0000 !  12.0000 !  407.5725 !  409.4233 !  411.0831 !
!------------+------------+------------+------------+------------+------------!
!   8.0000 !   20.0000 !   8.0000 !  409.3878 !  411.9871 !  418.2468 !
-------------------------------------------------------------------------------
-----------------------------------------------------
! VARY  1 ! VARY  2 ! VARY  3 ! TEMP24  !
! B1     ! B1     ! B1     !       !
! 8      ! 8      ! 1      !       !
! REAC-STA ! REAC-STA ! FEEDS   !       !
! STAGE1   ! STAGE2   ! STAGE   !       !
!        !        !        ! K     !
!        !        !        !       !
!============!============!============!============!
!   4.0000 !   16.0000 !   4.0000 !  417.4338 !
!   6.0000 !   18.0000 !   6.0000 !  422.8655 !
!   8.0000 !   20.0000 !   8.0000 !  441.3466 !
!  10.0000 !   22.0000 !  10.0000 !  422.2878 !
!  12.0000 !   24.0000 !  12.0000 !  417.2084 !
!------------+------------+------------+------------!
!   8.0000 !   20.0000 !   8.0000 !  441.3465 !
-----------------------------------------------------
```

```
 VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:
  VARIABLE        VALUE       UNITS
  --------       -----       -----
  DMEVP         0.999385
  DMELQ         0.994694
  TEMP16         407.342      K
  TEMP18         409.388      K
  TEMP20         411.987      K
  TEMP22         418.247      K
  TEMP24         441.347      K
SENSITIVITY BLOCK:  S-11
------------------------
 SAMPLED VARIABLES:
  DMEVP   : SENTENCE=COMPS VARIABLE=Y ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
  DMELQ   : SENTENCE=COMPS VARIABLE=X ID1=DIMET-01 ID2=1 IN UOS BLOCK B1
  TEMP20  : SENTENCE=PROFILE VARIABLE=TEMP ID1=20 IN UOS BLOCK B1

 VARIED VARIABLES:
  VARY   1: METHANOLMOLEFLOW IN STREAM 1 SUBSTREAM MIXED
  VARY   2: WATER MOLEFLOW IN STREAM 1 SUBSTREAM MIXED

 TABULATED VARIABLES:
  COLUMN  3: DMEVP
  COLUMN  4: DMELQ
  COLUMN  5: TEMP20

 CASE INFORMATION:
   CASE   1: "100%"
     VARY   1: 2.5000        VARY   2: 0.0
  CASE   2: "95%"
     VARY   1: 2.3750        VARY   2: 0.1250      CASE   3: "90%"
     VARY   1: 2.2500        VARY   2: 0.2500      CASE   4: "85%"
     VARY   1: 2.1250        VARY   2: 0.3750      CASE   5: "80%"
     VARY   1: 2.0000        VARY   2: 0.5000
-----------------------------------------------------------------------
! VARY  1 ! VARY  2 ! DMEVP    ! DMELQ    ! TEMP20   !
! 1       ! 1       !         !         !         !
! MIXED    ! MIXED    !         !         !         !
! METHANOL ! WATER MO !         !         !         !
! MOLEFLOW ! LEFLOW   !         !         !         !
! MOL/SEC  ! MOL/SEC  !         !         ! K       !
!         !         !         !         !         !
!============!============!============!============!============!
!   2.5000 !   0.0   !   0.9994 !   0.9947 !  411.9868 !
!   2.3750 !   0.1250 !   0.9880 !   0.9000 !  428.4625 !
!   2.2500 !   0.2500 !   0.9753 !   0.8002 !  445.8108 !
!   2.1250 !   0.3750 !   0.9624 !   0.7005 !  448.3492 !
!   2.0000 !   0.5000 !   0.9499 !   0.6009 !  448.5731 !
!------------+------------+------------+------------+------------!
!   2.5000 !   0.0   !   0.9994 !   0.9947 !  411.9869 !
-----------------------------------------------------------------------
```

VALUES OF ACCESSED FORTRAN VARIABLES ON MOST RECENT SIMULATION PASS:

VARIABLE	VALUE	UNITS
DMEVP	0.999385	
DMELQ	0.994693	
TEMP20	411.987	K

PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	ALIAS	NAME
WATER	C	H2O	WATER
METHANOL	C	CH4O	METHANOL
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER

U-O-S BLOCK SECTION

BLOCK: B1 MODEL: RADFRAC

INLETS	- 1	STAGE 8
OUTLETS	- 2	STAGE 1
	3	STAGE 25

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(MOL/SEC)	2.50000	2.50000	0.00000	0.177636E-14
MASS(KG/SEC)	0.801054E-01	0.801054E-01		0.207893E-14
ENTHALPY(WATT)	-596498.	-592474.		-0.674604E-02

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/SEC
PRODUCT STREAMS CO2E	0.572807E-01	KG/SEC
NET STREAMS CO2E PRODUCTION	0.572807E-01	KG/SEC
UTILITIES CO2E PRODUCTION	0.00000	KG/SEC
TOTAL CO2E PRODUCTION	0.572807E-01	KG/SEC

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	25
ALGORITHM OPTION	STANDARD
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	8.00000
DISTILLATE TO FEED RATIO	0.50000

**** REAC-STAGES SPECIFICATIONS ****

STAGE	TO STAGE	REACTIONS/CHEMISTRY ID
8	20	R-1

**** HOLD-UP SPECIFICATIONS ****

STAGE	TO STAGE	LIQUID HOLDUP	VAPOR HOLDUP
8	20	15.0000 KG	MISSING

***** REACTION PARAGRAPH R-1 *****

**** REACTION PARAMETERS ****

RXN NO.	TYPE	PHASE	CONC. BASIS	TEMP APP TO EQUIL K	CONVERSION
1	KINETIC	LIQUID	MOLAR		

** STOICHIOMETRIC COEFFICIENTS **

RXN NO.	WATER	METHANOL	DIMET-01
1	1.000	-2.000	1.000

**** PROFILES ****

P-SPEC STAGE 1 PRES, N/SQM 900,000.

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	2	3
COMPONENT:		
WATER	.48445E-07	1.0000
METHANOL	.50000	.50000
DIMET-01	1.0000	.22641E-07

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	K	313.604
BOTTOM STAGE TEMPERATURE	K	447.171
TOP STAGE LIQUID FLOW	MOL/SEC	10.0000
BOTTOM STAGE LIQUID FLOW	MOL/SEC	1.25000
TOP STAGE VAPOR FLOW	MOL/SEC	0.0
BOILUP VAPOR FLOW	MOL/SEC	5.46483
MOLAR REFLUX RATIO		8.00000
MOLAR BOILUP RATIO		4.37186
CONDENSER DUTY (W/O SUBCOOL)	WATT	-199,028.
REBOILER DUTY	WATT	203,052.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.89904E-06	STAGE= 4
BUBBLE POINT	0.28520E-05	STAGE= 3
COMPONENT MASS BALANCE	0.34987E-09	STAGE= 2 COMP=WATER
ENERGY BALANCE	0.18608E-05	STAGE= 4

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE K	PRESSURE N/SQM	ENTHALPY J/KMOL LIQUID	VAPOR	HEAT DUTY WATT
1	313.60	0.90000E+06	-0.20076E+09	-0.18308E+09	-.19903+06
2	314.96	0.90000E+06	-0.20198E+09	-0.18307E+09	
3	324.07	0.90000E+06	-0.21054E+09	-0.18306E+09	
7	398.66	0.90000E+06	-0.22723E+09	-0.19288E+09	
8	398.92	0.90000E+06	-0.22803E+09	-0.19317E+09	
9	400.67	0.90000E+06	-0.22901E+09	-0.19416E+09	
24	441.35	0.90000E+06	-0.27243E+09	-0.22897E+09	
25	447.17	0.90000E+06	-0.27322E+09	-0.23509E+09	.20305+06

STAGE	FLOW RATE MOL/SEC		FEED RATE MOL/SEC			PRODUCT RATE MOL/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	11.25	0.000				1.2500	
2	9.349	11.25					
3	6.879	10.60					
7	5.564	6.826					
8	8.912	6.814	2.5000				
9	8.815	7.662					
24	6.715	5.436					
25	1.250	5.465				1.2500	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/SEC		FEED RATE KG/SEC			PRODUCT RATE KG/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5174	0.000				.57493-01	
2	0.4248	0.5174					
3	0.2859	0.4823					
7	0.1773	0.2359					
8	0.2820	0.2348	.80105-01				
9	0.2760	0.2594					
24	0.1240	0.1120					
25	0.2261E-01	0.1014				.22612-01	

**** MOLE-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.48188E-07	0.53063E-02	0.99469
2	0.54866E-05	0.45032E-01	0.95496
3	0.39923E-03	0.32088	0.67872
7	0.19593E-01	0.97300	0.74106E-02
8	0.35958E-01	0.95625	0.77932E-02
9	0.58670E-01	0.93459	0.67417E-02
24	0.96793	0.32069E-01	0.22091E-06
25	0.99469	0.53063E-02	0.22521E-07

**** MOLE-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.40380E-09	0.61474E-03	0.99939
2	0.48188E-07	0.53063E-02	0.99469
3	0.48452E-05	0.40347E-01	0.95965
7	0.87480E-02	0.80310	0.18816
8	0.15998E-01	0.79548	0.18852
9	0.27245E-01	0.81599	0.15676
24	0.81493	0.18507	0.23720E-05
25	0.96181	0.38191E-01	0.26629E-06

**** K-VALUES ****

STAGE	WATER	METHANOL	DIMET-01
1	0.83796E-02	0.11585	1.0047
2	0.87829E-02	0.11783	1.0416
3	0.12136E-01	0.12574	1.4139
7	0.44649	0.82538	25.390
8	0.44492	0.83187	24.191
9	0.46438	0.87311	23.252
24	0.84193	5.7709	10.737
25	0.96694	7.1972	11.824

**** RATES OF GENERATION ****

MOL/SEC

STAG	WATER	METHANOL	DIMET-01
1	0.000	0.000	0.000
2	0.000	0.000	0.000
3	0.000	0.000	0.000
7	0.000	0.000	0.000
8	0.1117	-.2234	0.1117
9	0.1141	-.2282	0.1141
24	0.000	0.000	0.000
25	0.000	0.000	0.000

**** MASS-X-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.18875E-07	0.36966E-02	0.99630
2	0.21754E-05	0.31757E-01	0.96824
3	0.17307E-03	0.24741	0.75242
7	0.11075E-01	0.97821	0.10712E-01
8	0.20470E-01	0.96819	0.11345E-01
9	0.33754E-01	0.95633	0.99184E-02
24	0.94435	0.55649E-01	0.55116E-06
25	0.99060	0.93991E-02	0.57354E-07

**** MASS-Y-PROFILE ****

STAGE	WATER	METHANOL	DIMET-01
1	0.15793E-09	0.42765E-03	0.99957
2	0.18875E-07	0.36966E-02	0.99630
3	0.19183E-05	0.28411E-01	0.97159
7	0.45603E-02	0.74462	0.25082
8	0.83633E-02	0.73962	0.25202
9	0.14496E-01	0.77221	0.21329
24	0.71229	0.28771	0.53018E-05
25	0.93403	0.65965E-01	0.66131E-06

STREAM SECTION

1 2 3

STREAM ID	1	2	3
FROM :	----	B1	B1
TO :	B1	----	----
SUBSTREAM: MIXED			
PHASE:	LIQUID	LIQUID	LIQUID
COMPONENTS: MOL/SEC			
WATER	0.0	6.0236-08	1.2434
METHANOL	2.5000	6.6329-03	6.6329-03
DIMET-01	0.0	1.2434	2.8151-08
COMPONENTS: MOLE FRAC			
WATER	0.0	4.8188-08	0.9947
METHANOL	1.0000	5.3063-03	5.3063-03
DIMET-01	0.0	0.9947	2.2521-08
TOTAL FLOW:			
MOL/SEC	2.5000	1.2500	1.2500
KG/SEC	8.0105-02	5.7493-02	2.2612-02
CUM/SE	1.0100-04	9.1342-05	2.7182-05
STATE VARIABLES:			
TEMP K	298.0000	313.6037	447.1714
PRES N/SQM	9.0000+05	9.0000+05	9.0000+05
VFRAC	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0
ENTHALPY:			
J/KMOL	-2.3860+08	-2.0076+08	-2.7322+08
J/KG	-7.4464+06	-4.3648+06	-1.5104+07
WATT	-5.9650+05	-2.5095+05	-3.4153+05
ENTROPY:			
J/KMOL-K	-2.4091+05	-3.0914+05	-1.3077+05
J/KG-K	-7518.5980	-6721.2244	-7229.0324
DENSITY:			
KMOL/CUM	24.7517	13.6848	45.9869
KG/CUM	793.0991	629.4263	831.8904
AVG MW	32.0422	45.9946	18.0897

PROBLEM STATUS SECTION

BLOCK STATUS

****

* Calculations were completed with errors *
* *
* All Unit Operation blocks were completed normally *
* All streams were flashed normally *
* The following Sensitivity blocks were *
* completed with errors: *
* S-3 S-8 *

****

Appendix E

Aspen files: Traditional DME process and CD process simulation

```
DYNAMICS
   DYNAMICS RESULTS=ON
IN-UNITS ENG

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES OLD-DATABANK=YES

DESCRIPTION "
   General Simulation with English Units :
   F, psi, lb/hr, lbmol/hr, Btu/hr, cuft/hr.

   Property Method: None

   Flow basis for input: Mole

   Stream report composition: Mole flow
   "
DATABANKS PURE25  / AQUEOUS  / SOLIDS  / INORGANIC  /  &
      NOASPENPCD

PROP-SOURCES PURE25  / AQUEOUS  / SOLIDS  / INORGANIC

COMPONENTS
   METHANOL CH4O /
   WATER H2O /
   DIMET-01 C2H6O-1

FLOWSHEET
   BLOCK B1 IN=1 OUT=2
   BLOCK B2 IN=2 OUT=3 4
   BLOCK B3 IN=4 OUT=5 6
   BLOCK B4 IN=7 OUT=8 9

PROPERTIES NRTL

PROP-DATA NRTL-1
   IN-UNITS ENG
   PROP-LIST NRTL
   BPVAL METHANOL WATER -.6930000000 311.3767775 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL WATER METHANOL 2.732200000 -1111.083651 .3000000000  &
      0.0 0.0 0.0 76.98200338 212.0000023
   BPVAL METHANOL DIMET-01 0.0 1175.411331 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374
   BPVAL DIMET-01 METHANOL 0.0 -34.08695973 .2951000000 0.0  &
      0.0 0.0 32.00000374 32.00000374
```

```
STREAM 1
   SUBSTREAM MIXED TEMP=480. PRES=164.
   MASS-FLOW METHANOL 50000. <kg/hr>

STREAM 5
   SUBSTREAM MIXED TEMP=187.5 PRES=80. MASS-FLOW=13185.
   MOLE-FRAC METHANOL 0.933 / WATER 0.037 / DIMET-01 0.031

STREAM 7
   SUBSTREAM MIXED TEMP=298. <K> PRES=8. <atm>
   MASS-FLOW METHANOL 50000. <kg/hr>

BLOCK B2 RADFRAC
   PARAM NSTAGE=30
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 2 8
   PRODUCTS 3 1 L / 4 30 L
   P-SPEC 1 150.
   COL-SPECS MASS-D:F=0.69 MOLE-RR=15.

BLOCK B3 RADFRAC
   PARAM NSTAGE=10
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 4 8
   PRODUCTS 5 1 L / 6 10 L
   P-SPEC 1 80.
   COL-SPECS MASS-B:F=0.68 MOLE-RR=4.

BLOCK B4 RADFRAC
   PARAM NSTAGE=10
   COL-CONFIG CONDENSER=TOTAL
   FEEDS 7 6
   PRODUCTS 8 1 L / 9 10 L
   P-SPEC 1 8. <atm>
   COL-SPECS D:F=0.5 MOLE-RR=1.2
   REAC-STAGES 7 7 R-2

BLOCK B1 RGIBBS
   PARAM TEMP=480. PRES=164.

EO-CONV-OPTI

SENSITIVITY S-1
   DEFINE XDME MOLE-FRAC STREAM=4 SUBSTREAM=MIXED  &
      COMPONENT=DIMET-01
   DEFINE FDME BLOCK-VAR BLOCK=B2 VARIABLE=MASS-D  &
      SENTENCE=COL-RESULTS
   DEFINE XWATER MOLE-FRAC STREAM=6 SUBSTREAM=MIXED  &
      COMPONENT=WATER
   TABULATE 2 "XDME"
   VARY BLOCK-VAR BLOCK=B2 VARIABLE=MASS-D:F SENTENCE=COL-SPECS
   RANGE LOWER="0.5" UPPER="0.75" INCR="0.01"
```

```
STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

REACTIONS R-2 REAC-DIST
  REAC-DATA 1
  STOIC 1 METHANOL -2. / WATER 1. / DIMET-01 1.

REACTIONS R-1 GENERAL
  REAC-DATA 1 NAME=DEHY REAC-CLASS=EQUILIBRIUM
  STOIC 1 MIXED METHANOL -2. / WATER 1. / DIMET-01 1.

DISABLE
  SENSITIVITY S-1
```

User define kinetic subroutine fortran file

```
SUBROUTINE USRKNT      (N,    NCOMP,  NR,    NRL,    NRV,
   2                   T,    TLIQ,   TVAP,  P,      PHFRAC,
   3                   F,    X,      Y,     IDX,    NBOPST,
   4                   KDIAG, STOIC,  IHLBAS, HLDLIQ, TIMLIQ,
   5                   IHVBAS, HLDVAP, TIMVAP, NINT,  INT,
   6                   NREAL, REAL,   RATES, RATEL,  RATEV,
   7                   NINTB, INTB,   NREALB, REALB,  NIWORK,
   8                   IWORK, NWORK,  WORK)

    INTEGER NRL(3),IDX(NCOMP),  NBOPST(6),
   +      INT(NINT),   INTB(NINTB),
   +      IWORK(NIWORK),N,    KDIAG, IHLBAS,
   +      IHVBAS,NREAL
    REAL*8 PHFRAC(3),   X(NCOMP,3),  Y(NCOMP),
   +     STOIC(NCOMP,NR),    RATES(NCOMP),
   +     RATEL(1),    RATEV(NRV),
   +     REALB(NREALB),WORK(NWORK), T,    TLIQ,
   +     TVAP, P,    F,    HLDLIQ,TIMLIQ

    REAL*8 HLDVAP,TIMVAP
    INTEGER IMISS
    REAL*8 REAL(NREAL), RMISS
    REAL*8 Cm, Cw, Rate, Kw, Ks
    Cm=13*X(2,3)
    Cw=13*X(1,3)
    Ks=61200000*EXP(-98000.0/8.314/T)
    Kw=EXP(-6.46+2964.0/T)
    RATE=HLDLIQ*ks*Cm*Cm/(Kw*Cw+Cm)*(Kw*Cw+Cm)
    RATES(3)=RATE
    RATES(1)=RATE
    RATES(2)=-RATE

    RETURN
    END
```

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
1	----	B1	7	----	B4
2	B1	B2	3	B2	----
4	B2	B3	5	B3	----
6	B3	----	8	B4	----
9	B4	----			

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
B1	1	2
B2	2	3 4
B3	4	5 6
B4	7	8 9

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
B4 B1 B2 B3

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (LBMOL/HR)				
METHANOL	6880.38	385.756	-6494.63	-0.513897E-08
WATER	0.00000	3247.31	3247.31	-0.622658E-06
DIMET-01	0.00000	3247.31	3247.31	0.633547E-06
TOTAL BALANCE				
MOLE(LBMOL/HR)	6880.38	6880.38	-0.502252E-10	0.264373E-15
MASS(LB/HR)	220462.	220462.		0.259544E-06
ENTHALPY(BTU/HR)	-0.632671E+09	-0.701420E+09		0.980141E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	149600.	LB/HR
NET STREAMS CO2E PRODUCTION	149600.	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	149600.	LB/HR

COMPONENTS

ID	TYPE	ALIAS	NAME
METHANOL	C	CH4O	METHANOL
WATER	C	H2O	WATER
DIMET-01	C	C2H6O-1	DIMETHYL-ETHER

U-O-S BLOCK SECTION

BLOCK: B1 MODEL: RGIBBS

INLET STREAM: 1
OUTLET STREAM: 2
PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(LBMOL/HR)	3440.19	3440.19	-0.502252E-10	0.132187E-15
MASS(LB/HR)	110231.	110231.		0.101650E-13
ENTHALPY(BTU/HR)	-0.279779E+09	-0.294076E+09		0.486156E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	70418.7	LB/HR
NET STREAMS CO2E PRODUCTION	70418.7	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	70418.7	LB/HR

*** INPUT DATA ***

EQUILIBRIUM SPECIFICATIONS:
ONLY CHEMICAL EQUILIBRIUM IS CONSIDERED, THE FLUID PHASE IS VAPOR

SYSTEM TEMPERATURE	F	480.00
TEMPERATURE FOR FREE ENERGY EVALUATION	F	480.00
SYSTEM PRESSURE	PSIA	164.00

FLUID PHASE SPECIES IN PRODUCT LIST:
METHANOL WATER DIMET-01

ATOM MATRIX:

ELEMENT	H	C	O
METHANOL	4.00	1.00	1.00
WATER	2.00	0.00	1.00
DIMET-01	6.00	2.00	1.00

*** RESULTS ***

TEMPERATURE	F	480.00
PRESSURE	PSIA	164.00
HEAT DUTY	BTU/HR	-0.14297E+08
VAPOR FRACTION		1.0000
NUMBER OF FLUID PHASES		1

FLUID PHASE MOLE FRACTIONS:

PHASE	VAPOR
OF TYPE	VAPOR
PHASE FRACTION	1.000000
PLACED IN STREAM	2
METHANOL	0.1113586
DIMET-01	0.4443207
WATER	0.4443207

LBMOL/HR 3440.190

BLOCK: B2 MODEL: RADFRAC

INLETS	- 2	STAGE	8
OUTLETS	- 3	STAGE	1
	4	STAGE	30

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	3440.19	3440.19	0.00000
MASS(LB/HR)	110231.	110231.	0.518827E-06
ENTHALPY(BTU/HR	-0.294076E+09	-0.349065E+09	0.157533

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	70418.7	LB/HR
PRODUCT STREAMS CO2E	70418.6	LB/HR
NET STREAMS CO2E PRODUCTION	-0.947790E-01	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	-0.947790E-01	LB/HR

****

**** INPUT DATA ****

****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	30
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	15.0000
MASS DISTILLATE TO FEED RATIO	0.69000

**** PROFILES ****

P-SPEC	STAGE 1 PRES, PSIA	150.000

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	3	4
COMPONENT:		
METHANOL	.45894	.54106
WATER	.26446E-03	.99974
DIMET-01	1.0000	0.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	120.812
BOTTOM STAGE TEMPERATURE	F	325.442
TOP STAGE LIQUID FLOW	LBMOL/HR	25,571.5
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	1,735.42
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	12,001.0
MOLAR REFLUX RATIO		15.0000
MOLAR BOILUP RATIO		6.91531
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.235942+09
REBOILER DUTY	BTU/HR	0.180952+09

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.47294E-04	STAGE= 3
BUBBLE POINT	0.54651E-04	STAGE= 2
COMPONENT MASS BALANCE	0.99932E-05	STAGE= 7 COMP=DIMET-01
ENERGY BALANCE	0.13009E-03	STAGE= 3

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS
FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	ENTHALPY PRESSURE PSIA	BTU/LBMOL LIQUID	VAPOR	HEAT DUTY BTU/HR
1	120.81	150.00	-87276.	-78547.	-.23594+09
2	157.65	150.00	-96243.	-78626.	
3	256.04	150.00	-97615.	-81847.	
6	277.94	150.00	-99141.	-84402.	
7	280.65	150.00	-0.10101E+06	-85142.	
8	286.34	150.00	-0.10093E+06	-85959.	
29	303.31	150.00	-0.11001E+06	-89930.	
30	325.44	150.00	-0.11541E+06	-94153.	.18095+09

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.2728E+05	0.000				1704.7663	
2	0.1575E+05	0.2728E+05					
3	0.1643E+05	0.1746E+05					
6	0.1659E+05	0.1855E+05					
7	0.1542E+05	0.1830E+05			3440.1904		
8	0.1555E+05	0.1368E+05					
29	0.1374E+05	0.1287E+05					
30	1735.	0.1200E+05				1735.4241	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1217E+07	0.000				.76059+05	
2	0.5594E+06	0.1217E+07					
3	0.5254E+06	0.6355E+06					
6	0.5069E+06	0.6018E+06					
7	0.4524E+06	0.5830E+06	.11023+06				
8	0.4552E+06	0.4182E+06					
29	0.3214E+06	0.3517E+06					
30	0.3417E+05	0.2872E+06				.34172+05	

**** MOLE-X-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.10313	0.23712E-03	0.89663
2	0.73558	0.83774E-02	0.25604
3	0.96411	0.20650E-01	0.15240E-01
6	0.88485	0.11083	0.43183E-02
7	0.79663	0.19794	0.54369E-02
8	0.80176	0.19788	0.35900E-03
29	0.38355	0.61645	0.23621E-27
30	0.11944	0.88056	0.31155E-28

**** MOLE-Y-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.13743E-01	0.25785E-05	0.98625
2	0.10313	0.23712E-03	0.89663
3	0.67382	0.75825E-02	0.31860
6	0.85681	0.57342E-01	0.85851E-01
7	0.81202	0.10053	0.87448E-01
8	0.88253	0.11135	0.61266E-02
29	0.66398	0.33602	0.20607E-26
30	0.42175	0.57825	0.26586E-27

**** K-VALUES ****

STAGE	METHANOL	WATER	DIMET-01
1	0.13326	0.10874E-01	1.1000
2	0.14020	0.28305E-01	3.5021
3	0.69887	0.36708	20.910
6	0.96831	0.51737	19.881
7	1.0193	0.50790	16.084
8	1.1007	0.56271	17.066
29	1.7311	0.54510	8.7244
30	3.5310	0.65669	8.5333

**** MASS-X-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.74068E-01	0.95746E-04	0.92584
2	0.66363	0.42494E-02	0.33212
3	0.96640	0.11638E-01	0.21963E-01
6	0.92813	0.65363E-01	0.65124E-02
7	0.86994	0.12153	0.85364E-02
8	0.87765	0.12178	0.56501E-03
29	0.52531	0.47469	0.46512E-27
30	0.19436	0.80564	0.72892E-28

**** MASS-Y-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.95988E-02	0.10126E-05	0.99040
2	0.74068E-01	0.95746E-04	0.92584
3	0.59307	0.37523E-02	0.40318
6	0.84625	0.31842E-01	0.12191
7	0.81670	0.56847E-01	0.12645
8	0.92514	0.65626E-01	0.92339E-02
29	0.77849	0.22151	0.34739E-26
30	0.56469	0.43531	0.51179E-27

BLOCK: B3 MODEL: RADFRAC

INLETS	- 4	STAGE	8
OUTLETS	- 5	STAGE	1
	6	STAGE	10

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(LBMOL/HR)	1735.42	1735.42	-0.131019E-15
MASS(LB/HR)	34171.6	34171.6	0.845396E-09
ENTHALPY(BTU/HR)	-0.200281E+09	-0.201418E+09	0.564727E-02

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	LB/HR
PRODUCT STREAMS CO2E	0.00000	LB/HR
NET STREAMS CO2E PRODUCTION	0.00000	LB/HR
UTILITIES CO2E PRODUCTION	0.00000	LB/HR
TOTAL CO2E PRODUCTION	0.00000	LB/HR

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	10
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	4.00000
MASS BOTTOMS TO FEED RATIO	0.68000

**** PROFILES ****

P-SPEC	STAGE 1	PRES, PSIA	80.0000

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	5	6
COMPONENT:		
METHANOL	.99629	.37061E-02
WATER	.15684	.84316

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	257.217
BOTTOM STAGE TEMPERATURE	F	311.905
TOP STAGE LIQUID FLOW	LBMOL/HR	1,784.76
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	1,289.23
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	2,067.27
MOLAR REFLUX RATIO		4.00000
MOLAR BOILUP RATIO		1.60349
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.348707+08
REBOILER DUTY	BTU/HR	0.337331+08

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.21756E-05	STAGE= 2
BUBBLE POINT	0.16415E-03	STAGE= 2
COMPONENT MASS BALANCE	0.23230E-05	STAGE= 8 COMP=METHANOL
ENERGY BALANCE	0.85745E-04	STAGE= 2

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

			ENTHALPY		
STAGE	TEMPERATURE	PRESSURE	BTU/LBMOL		HEAT DUTY
	F	PSIA	LIQUID	VAPOR	BTU/HR
1	257.22	80.000	-0.10950E+06	-89323.	-.34871+08
2	279.44	80.000	-0.11610E+06	-93870.	
3	298.89	80.000	-0.11786E+06	-98379.	
6	305.34	80.000	-0.11814E+06	-0.10009E+06	
7	305.36	80.000	-0.11814E+06	-0.10010E+06	
8	306.36	80.000	-0.11817E+06	-0.10038E+06	
9	310.83	80.000	-0.11831E+06	-0.10165E+06	
10	311.90	80.000	-0.11833E+06	-0.10197E+06	.33733+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	2231.	0.000				446.1891	
2	1687.	2231.					
3	1693.	2133.					
6	1701.	2147.					
7	1701.	2147.			110.5920		
8	3344.	2036.	1624.8320				
9	3357.	2055.					
10	1289.	2067.				1289.2349	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5467E+05	0.000				.10935+05	
2	0.3367E+05	0.5467E+05					
3	0.3136E+05	0.4460E+05					
6	0.3103E+05	0.4197E+05					
7	0.3104E+05	0.4197E+05			2605.9655		
8	0.6090E+05	0.3937E+05	.31566+05				
9	0.6061E+05	0.3766E+05					
10	0.2324E+05	0.3737E+05				.23237+05	

**** MOLE-X-PROFILE ****

STAGE	METHANOL	WATER
1	0.46283	0.53717
2	0.13830	0.86170
3	0.36390E-01	0.96361
6	0.16681E-01	0.98332
7	0.16630E-01	0.98337
8	0.13945E-01	0.98606
9	0.30116E-02	0.99699
10	0.59586E-03	0.99940

**** MOLE-Y-PROFILE ****

STAGE	METHANOL	WATER
1	0.72553	0.27447
2	0.46283	0.53717
3	0.20618	0.79382
6	0.10970	0.89030
7	0.10941	0.89059
8	0.93814E-01	0.90619
9	0.22321E-01	0.97768
10	0.45182E-02	0.99548

**** K-VALUES ****

STAGE	METHANOL	WATER
1	1.5676	0.51095
2	3.3451	0.62343
3	5.6653	0.82381
6	6.5765	0.90540
7	6.5792	0.90565
8	6.7277	0.91900
9	7.4116	0.98063
10	7.5827	0.99608

**** MASS-X-PROFILE ****

STAGE	METHANOL	WATER
1	0.60513	0.39487
2	0.22207	0.77793
3	0.62940E-01	0.93706
6	0.29288E-01	0.97071
7	0.29201E-01	0.97080
8	0.24536E-01	0.97546
9	0.53440E-02	0.99466
10	0.10593E-02	0.99894

**** MASS-Y-PROFILE ****

STAGE	METHANOL	WATER
1	0.82461	0.17539
2	0.60513	0.39487
3	0.31598	0.68402
6	0.17976	0.82024
7	0.17932	0.82068
8	0.15550	0.84450
9	0.39022E-01	0.96098
10	0.80080E-02	0.99199

U-O-S BLOCK SECTION

BLOCK: B4 MODEL: RADFRAC

INLETS	- 7	STAGE 6
OUTLETS	- 8	STAGE 1
	9	STAGE 10

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	GENERATION	RELATIVE DIFF.
TOTAL BALANCE				
MOLE(LBMOL/HR)	3440.19	3440.19	0.00000	0.132187E-15
MASS(LB/HR)	110231.	110231.		0.264026E-15
ENTHALPY(BTU/HR)	-0.352892E+09	-0.351218E+09		-0.474492E-02

****
**** INPUT DATA ****
****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	10
ALGORITHM OPTION	STANDARD
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	1.20000
DISTILLATE TO FEED RATIO	0.50000

**** REAC-STAGES SPECIFICATIONS ****

STAGE	TO STAGE	REACTIONS/CHEMISTRY ID
7	7	R-2

***** REACTION PARAGRAPH R-2 *****

**** REACTION PARAMETERS ****

RXN NO.	TYPE	PHASE	CONC. BASIS	TEMP APP TO EQUIL F	CONVERSION
1	EQUILIBRIUM	LIQUID	MOLE-GAMMA	0.0000	

** STOICHIOMETRIC COEFFICIENTS **

RXN NO.	METHANOL	WATER	DIMET-01
1	-2.000	1.000	1.000

**** PROFILES ****

P-SPEC	STAGE 1	PRES, PSIA	117.568

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	8	9
COMPONENT:		
METHANOL	.73417	.26583
WATER	.10850E-07	1.0000
DIMET-01	.99964	.36255E-03

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	F	97.3855
BOTTOM STAGE TEMPERATURE	F	339.370
TOP STAGE LIQUID FLOW	LBMOL/HR	2,064.11
BOTTOM STAGE LIQUID FLOW	LBMOL/HR	1,720.10
TOP STAGE VAPOR FLOW	LBMOL/HR	0.0
BOILUP VAPOR FLOW	LBMOL/HR	1,927.31
MOLAR REFLUX RATIO		1.20000
MOLAR BOILUP RATIO		1.12046
CONDENSER DUTY (W/O SUBCOOL)	BTU/HR	-0.290133+08
REBOILER DUTY	BTU/HR	0.306877+08

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.21425E-04	STAGE= 6	
BUBBLE POINT	0.83380E-04	STAGE= 5	
COMPONENT MASS BALANCE	0.89075E-07	STAGE= 3	COMP=WATER
ENERGY BALANCE	0.68982E-05	STAGE= 6	

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE F	PRESSURE PSIA	ENTHALPY BTU/LBMOL LIQUID	VAPOR	HEAT DUTY BTU/HR
1	97.386	117.57	-86491.	-78826.	-.29013+08
2	97.956	117.57	-86616.	-78824.	
3	100.77	117.57	-87234.	-78817.	
5	153.13	117.57	-98802.	-78862.	
6	197.75	117.57	-0.10176E+06	-79781.	
7	264.00	117.57	-0.11457E+06	-83837.	
9	336.77	117.57	-0.11763E+06	-0.10073E+06	
10	339.37	117.57	-0.11769E+06	-0.10165E+06	.30688+08

STAGE	FLOW RATE LBMOL/HR		FEED RATE LBMOL/HR			PRODUCT RATE LBMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	3784.	0.000				1720.0952	
2	2027.	3784.					
3	1870.	3747.					
5	918.5	3136.					
6	4961.	2639.	3440.1904				
7	3673.	3241.					
9	3647.	1912.					
10	1720.	1927.				1720.0952	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE LB/HR		FEED RATE LB/HR			PRODUCT RATE LB/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1743E+06	0.000				.79216+05	
2	0.9310E+05	0.1743E+06					
3	0.8467E+05	0.1723E+06					
5	0.3097E+05	0.1391E+06					
6	0.1523E+06	0.1102E+06	.11023+06				
7	0.7759E+05	0.1213E+06					
9	0.6607E+05	0.3651E+05					
10	0.3102E+05	0.3505E+05				.31015+05	

**** MOLE-X-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.11357E-02	0.10842E-07	0.99886
2	0.10587E-01	0.14359E-05	0.98941
3	0.57057E-01	0.97944E-04	0.94285
5	0.75578	0.62478E-01	0.18174
6	0.72599	0.18483	0.89187E-01
7	0.22227E-01	0.87798	0.99794E-01
9	0.18273E-02	0.99559	0.25850E-02
10	0.41122E-03	0.99923	0.36226E-03

**** MOLE-Y-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.12130E-03	0.80944E-10	0.99988
2	0.11357E-02	0.10842E-07	0.99886
3	0.62487E-02	0.78178E-06	0.99375
5	0.11765	0.22479E-02	0.88010
6	0.26383	0.21749E-01	0.71442
7	0.50444E-01	0.28292	0.66664
9	0.13187E-01	0.95488	0.31931E-01
10	0.30912E-02	0.99234	0.45688E-02

**** K-VALUES ****

STAGE	METHANOL	WATER	DIMET-01
1	0.10680	0.74659E-02	1.0010
2	0.10728	0.75507E-02	1.0096
3	0.10952	0.79819E-02	1.0540
5	0.15568	0.35980E-01	4.8422
6	0.36342	0.11768	8.0098
7	2.2696	0.32224	6.6799
9	7.2168	0.95911	12.352
10	7.5170	0.99311	12.612

**** RATES OF GENERATION ****

LBMOL/HR

STAGE	METHANOL	WATER	DIMET-01
1	0.000	0.000	0.000
2	0.000	0.000	0.000
3	0.000	0.000	0.000
5	0.000	0.000	0.000
6	0.000	0.000	0.000
7	-3438.	1719.	1719.
9	0.000	0.000	0.000
10	0.000	0.000	0.000

**** MASS-X-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.79020E-03	0.42411E-08	0.99921
2	0.73871E-02	0.56331E-06	0.99261
3	0.40389E-01	0.38980E-04	0.95957
5	0.71828	0.33384E-01	0.24833
6	0.75771	0.10846	0.13383
7	0.33711E-01	0.74868	0.21761
9	0.32325E-02	0.99019	0.65747E-02
10	0.73076E-03	0.99834	0.92557E-03

**** MASS-Y-PROFILE ****

STAGE	METHANOL	WATER	DIMET-01
1	0.84367E-04	0.31654E-10	0.99992
2	0.79020E-03	0.42411E-08	0.99921
3	0.43544E-02	0.30630E-06	0.99565
5	0.84992E-01	0.91300E-03	0.91410
6	0.20245	0.93829E-02	0.78817
7	0.43189E-01	0.13619	0.82062
9	0.22128E-01	0.90084	0.77033E-01
10	0.54461E-02	0.98298	0.11573E-01

STREAM SECTION

1 2 3 4 5

STREAM ID	1	2	3	4	5
FROM :	----	B1	B2	B2	B3
TO :	B1	B2	----	B3	----
SUBSTREAM: MIXED					
PHASE:	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR					
METHANOL	3440.1904	383.0949	175.8164	207.2786	206.5104
WATER	0.0	1528.5478	0.4042	1528.1455	239.6788
DIMET-01	0.0	1528.5478	1528.5457	5.4068-26	0.0
COMPONENTS: MOLE FRAC					
METHANOL	1.0000	0.1114	0.1031	0.1194	0.4628
WATER	0.0	0.4443	2.3712-04	0.8806	0.5372
DIMET-01	0.0	0.4443	0.8966	3.1155-29	0.0
COMPONENTS: LB/HR					
METHANOL	1.1023+05	1.2275+04	5633.5365	6641.6531	6617.0383
WATER	0.0	2.7537+04	7.2824	2.7530+04	4317.8810
DIMET-01	0.0	7.0419+04	7.0419+04	2.4908-24	0.0
COMPONENTS: MASS FRAC					
METHANOL	1.0000	0.1114	7.4068-02	0.1944	0.6051
WATER	0.0	0.2498	9.5746-05	0.8056	0.3949
DIMET-01	0.0	0.6388	0.9258	7.2892-29	0.0
TOTAL FLOW:					
LBMOL/HR	3440.1904	3440.1904	1704.7663	1735.4241	446.1892
LB/HR	1.1023+05	1.1023+05	7.6059+04	3.4172+04	1.0935+04
CUFT/HR	2.1153+05	2.1153+05	1941.1113	693.6608	238.4887
STATE VARIABLES:					
TEMP F	480.0000	480.0000	120.8120	325.4418	257.2171
PRES PSIA	164.0000	164.0000	150.0000	150.0000	80.0000
VFRAC	1.0000	1.0000	0.0	0.0	0.0
LFRAC	0.0	0.0	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
BTU/LBMOL	-8.1327+04	-8.5482+04	-8.7276+04	-1.1541+05	-1.0950+05
BTU/LB	-2538.1158	-2667.8130	-1956.1639	-5861.0227	-4468.0623
BTU/HR	-2.7978+08	-2.9408+08	-1.4878+08	-2.0028+08	-4.8858+07
ENTROPY:					
BTU/LBMOL-R	-28.8033	-28.8669	-70.7692	-33.1850	-40.4121
BTU/LB-R	-0.8989	-0.9009	-1.5862	-1.6853	-1.6490
DENSITY:					
LBMOL/CUFT	1.6263-02	1.6263-02	0.8782	2.5018	1.8709
LB/CUFT	0.5211	0.5211	39.1835	49.2627	45.8509
AVG MW	32.0422	32.0422	44.6158	19.6906	24.5074

6 7 8 9

STREAM ID	6	7	8	9
FROM :	B3	----	B4	B4
TO :	----	B4	----	----
SUBSTREAM: MIXED				
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: LBMOL/HR				
METHANOL	0.7682	3440.1904	1.9536	0.7073
WATER	1288.4667	0.0	1.8649-05	1718.7647
DIMET-01	0.0	0.0	1718.1416	0.6231
COMPONENTS: MOLE FRAC				
METHANOL	5.9586-04	1.0000	1.1357-03	4.1122-04
WATER	0.9994	0.0	1.0842-08	0.9992
DIMET-01	0.0	0.0	0.9989	3.6226-04
COMPONENTS: LB/HR				
METHANOL	24.6147	1.1023+05	62.5964	22.6647
WATER	2.3212+04	0.0	3.3597-04	3.0964+04
DIMET-01	0.0	0.0	7.9153+04	28.7070
COMPONENTS: MASS FRAC				
METHANOL	1.0593-03	1.0000	7.9020-04	7.3076-04
WATER	0.9989	0.0	4.2411-09	0.9983
DIMET-01	0.0	0.0	0.9992	9.2557-04
TOTAL FLOW:				
LBMOL/HR	1289.2349	3440.1904	1720.0952	1720.0952
LB/HR	2.3237+04	1.1023+05	7.9216+04	3.1015+04
CUFT/HR	434.5826	2226.3716	1995.2953	592.6961
STATE VARIABLES:				
TEMP F	311.9050	76.7300	97.3855	339.3696
PRES PSIA	80.0000	117.5676	117.5676	117.5676
VFRAC	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0
ENTHALPY:				
BTU/LBMOL	-1.1833+05	-1.0258+05	-8.6491+04	-1.1769+05
BTU/LB	-6565.4847	-3201.3819	-1878.0698	-6527.2359
BTU/HR	-1.5256+08	-3.5289+08	-1.4877+08	-2.0244+08
ENTROPY:				
BTU/LBMOL-R	-32.1232	-57.5409	-74.3518	-31.3677
BTU/LB-R	-1.7823	-1.7958	-1.6145	-1.7396
DENSITY:				
LBMOL/CUFT	2.9666	1.5452	0.8621	2.9022
LB/CUFT	53.4690	49.5116	39.7013	52.3293
AVG MW	18.0236	32.0422	46.0531	18.0312

PROBLEM STATUS SECTION

BLOCK STATUS

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* Calculations were completed normally

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* All Unit Operation blocks were completed normally

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* All streams were flashed normally

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* All Sensitivity blocks were completed normally

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