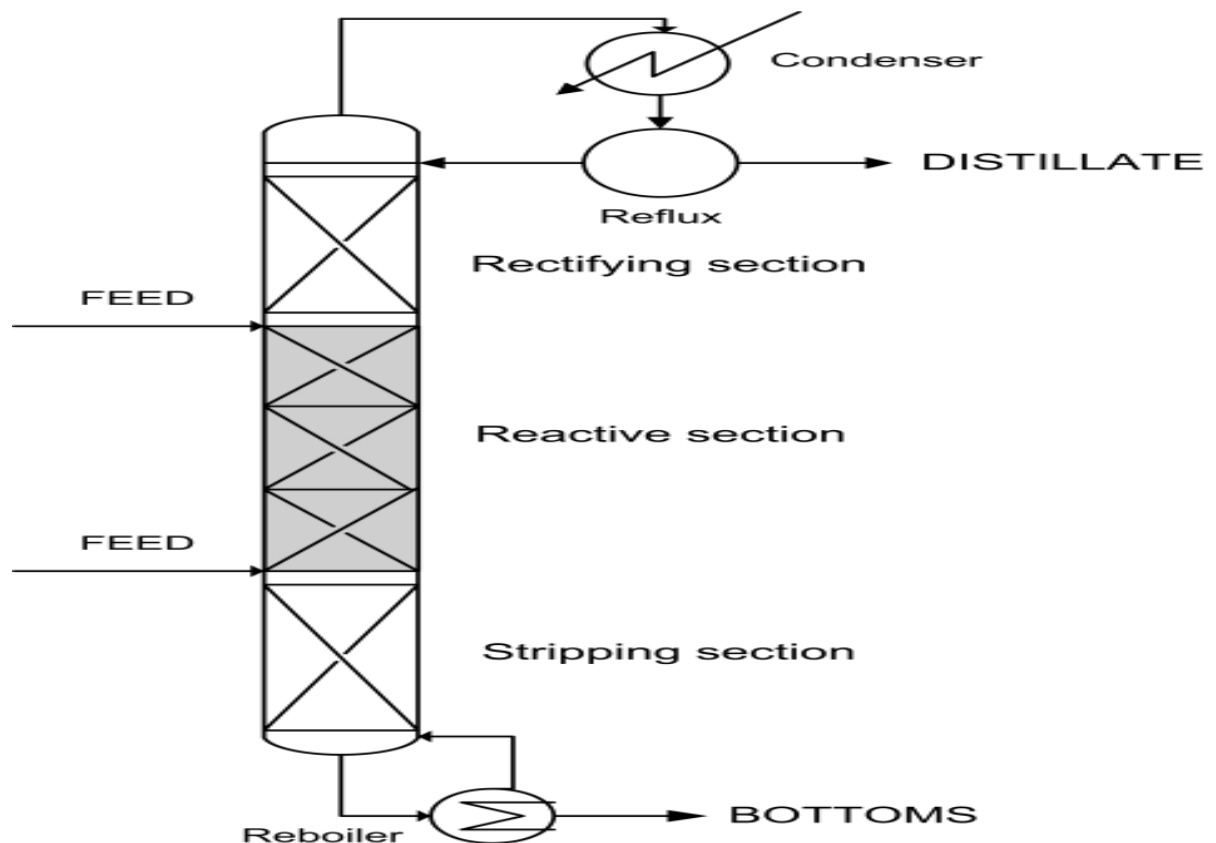


# REACTIVE DISTILLATION-A Novel Process Intensification Technique

- Distillation is a method of separating mixtures based on differences in volatility of components in a boiling liquid mixture,
- Reactive Distillation (RD) is a combination of reaction and distillation in a single vessel, Separation of the product from the reaction mixture does not need a separate distillation step, which saves energy, The product is usually significantly lower-boiling than its reactants, it is vaporized and removed from the reaction mixture.



## BENEFITS

- Increased speed
- Lower costs – reduced equipment use, energy use and handling
- Less waste and fewer byproducts
- Improved product quality– reducing opportunity for degradation because of less heat

## DIFFICULTIES

The conditions in the reactive column are suboptimal both as a chemical reactor and as a distillation column, since the reactive column combines these. The introduction of an in situ separation process in the reaction zone or vice versa leads to complex interactions between vapor–liquid equilibrium, mass transfer rates, diffusion and chemical kinetics, which poses a great challenge for design and synthesis of these systems. Side reactors, where a separate column feeds a reactor and vice versa, are better for some reactions, if the optimal conditions of distillation and reaction differ too much.

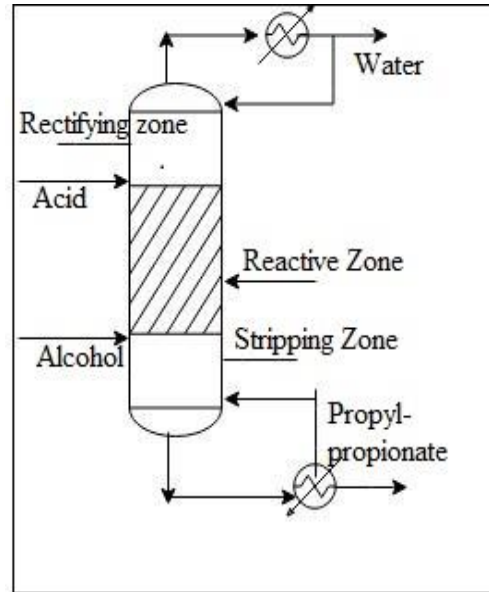
# APPLICATION

Reactive distillation can be used with a wide variety of chemistries, including the following:

- Acetylation
- Aldol condensation
- Alkylation
- Amination
- Dehydration
- Esterification
- Etherification
- Hydrolysis
- Isomerization
- Oligomerization
- Transesterification
- Hydrodesulfurization of light oil fractions

# PROCEDURE

1. Clean feed tank, reboiler and check that rotameter, condenser and pumps are working properly.
2. Fill the feed tank. Feed tank 1 is dedicated for alcohol while feed tank 2 is dedicated for second reactant which may be acetic acid, TAA, TBA etc. as the case may be.
3. Fill the chiller and jacket of feed tank with water.
4. Now fill the reboiler approximately 2.5 ltr with lower boiling point (more volatile) reactant which is generally alcohol.
5. Now start the heater for reboiler, feed tanks.
6. Set the reboiler temperature closer to the boiling point of component which is filled in reboiler.
7. Similarly set the feed temperature lower than the boiling point of respective component.
8. Start noting the sensor temperature readings and observe the column.
9. Start feeding the higher boiling point (less volatile) feed at top of reactive zone when the temperature above this section is approximately closer to the boiling point of higher volatile component.
10. Let the reaction to proceed and product to be collected at top.
11. Take a sample and analyse for concentration measurement.
12. Now start the reflux and again let the system to come under steady state so as product start collecting at the top.
13. Again take a sample to check the purity after reflux.



## DIFFERENT CASE STUDIES

- METHYL ACETATE SYNTHESIS IN PILOT REACTIVE DISTILLATION USING AMBERLYST 15 WET**  
**Methyl acetate**, also known as **MeOAc**, **acetic acid methyl ester** or **methyl ethanoate**, is a carboxylate ester with the formula  $\text{CH}_3\text{COOCH}_3$ . It is a flammable liquid with a characteristically pleasant smell reminiscent of some glues and nail polish removers. Methyl acetate is occasionally used as a solvent, being weakly polar and lipophilic, but its close relative ethyl acetate is a more common solvent being less toxic and less soluble in water. It is synthesized using acetic acid and methanol as raw materials. The reaction proceed as follow:



$$r = m_{\text{cat}}(k_1 * x_{\text{meOAc}} * x_{\text{H}_2\text{O}} - k_2 * x_{\text{HOAc}} * x_{\text{MeOH}})$$

$$k_1 = k_1^0 \exp(-E_1/RT)$$

$$k_2 = k_2^0 \exp(-E_2/RT)$$

Where  $m_{\text{cat}}$  is the mass of catalyst=500gms

T ranges from 323k to 373k

R is universal gas constant=8.314j/gmmol<sup>0</sup>k

E1, E2 are the activation energy, j/mole<sup>0</sup>k

E1=53340

E2=30363

$k_1^0$ ,  $k_2^0$  are the standard rate constant, gmole/sec

$k_1^0=13325$

$k_2^0=17.67$

$x_{\text{MeOH}}=0.99$ (initial concentration of methanol)

$x_{\text{HOAc}}=0.99$ (initial concentration of acetic acid)

$x_{\text{meOAc}}$  ranges from 0-1(product purity)

$x_{\text{H}_2\text{O}}$  ranges from 0-1(bottom product purity)

TABLE 1: OPERATING CONDITIONS

PARAMETERS	VALUE
PRESSURE	ATMOSPHERIC
REBOILER DUTY	2 KW
FEED 1 ( METHANOL)	AT BOTTOM OF REACTIVE ZONE
FEED 2 (ACETIC ACID)	AT TOP OF REACTIVE ZONE
FEED 1 TEMPERATURE	60 C
FEED 2 TEMPERATURE	80 C
FEED 1 FLOW RATE	0.02 L/MIN
FEED 2 FLOW RATE	0.02 L/MIN
REFLUX RATE	0.15 l/min
DISTILLATE FLOW RATE	0.05 ml/min
REFLUX RATIO	3
INITIAL REBOILER HOLD UP	1 Ltr
MAXIMUM REBOILER CAPACITY	2 LTR
TOTAL SEGMENT	8
REBOILER	10 <sup>TH</sup> SEGMENT
CONDENSER TYPE	VERTICAL
FIRST TIME TO STEADY STATE	30 min
SECOND TIME TO STEADY STATE	55 min
FINAL TIME TO STEADY STATE	85 min
HEIGHT OF COLUMN	3 METER
PACKING IN REACTIVE ZONE	AMBERLYST 15 WET
PACKING IN RECTIFYING + STRIPPING ZONE	KATAPAK S

TABLE 2: EXPERIMENTAL TEMPERATURE DETAIL WITH TIME

TIME ↓ SEGMENT(Temp) →	T1	T2	T3	T4	T5	T6	T7	T8	T9	REBOILER TEMP
5 min	32	37	33	38	37	34	34	30	32	50
10 min	32	37	32	37	37	35	34	30	32	57
15 min	61	37	32	38	38	35	34	31	33	64.5
20 min	62	63	60	38	38	35	34	31	33	65
25 min	61	63	60	66	64	35	34	31	32	65.2
30 min	62	64	60	66	67	63	56	31	53	65.5
35 min	62	64	61	66	67	62	56	55	53	65.5
40 min	62	64	62	67	77	62	56	53	55	65.7
45 min	64	66	64	70	75	65	53	49	54	68
50 min	65	68	64	70	75	66	57	51	49	68.5
55 min	65	68	63	67	73	66	58	53	55	68.5
60 min	65	67	63	70	73	66	58	55	55	70
65 min	65	68	63	70	73	66	58	55	55	69
70 min	67	69	65	67	73	68	60	57	57	70
75 min	66	67	65	67	76	63	57	54	56	70
80 min	68	67	64	69	70	63	57	54	58	72
85 min	66	67	65	67	70	63	54	53	57	72.5
90 min	66	66	65	68	69	64	57	52	57	72.5
95 min	65	67	64	68	70	64	55	53	56	72.7
100 min	66	67	65	68	70	63	57	53	57	73

METHYL ACETATE SIMULATION IN ASPEN PLUS: OPERATING CONDITIONS ARE SAME AS OF EXPERIMENT AS DETAILED IN TABLE 1

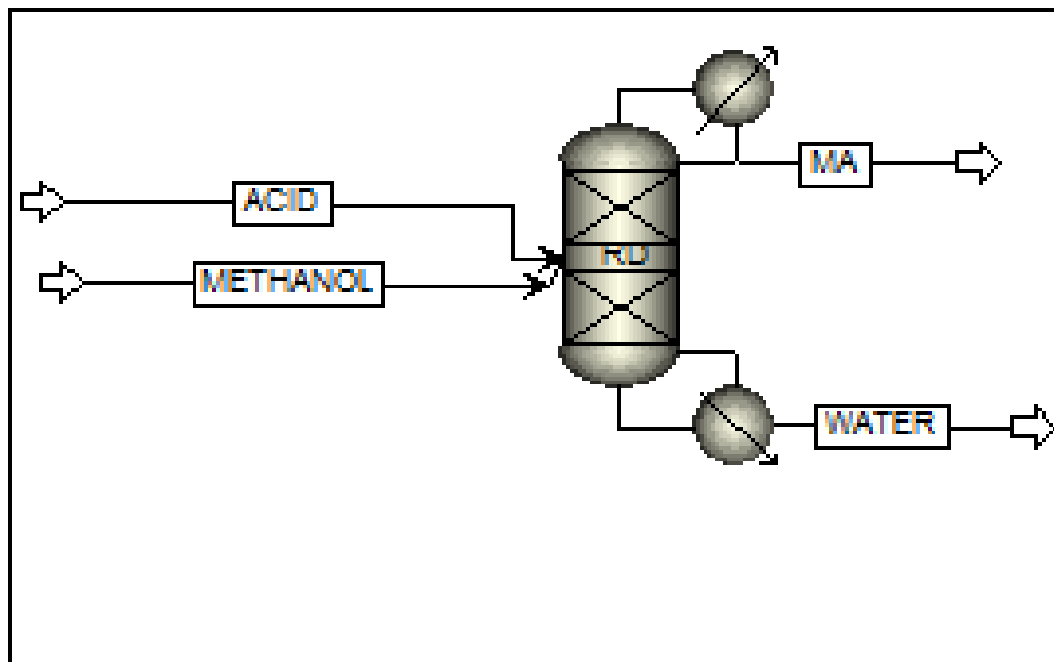


Fig.1 Schematic of Methyl acetate synthesis

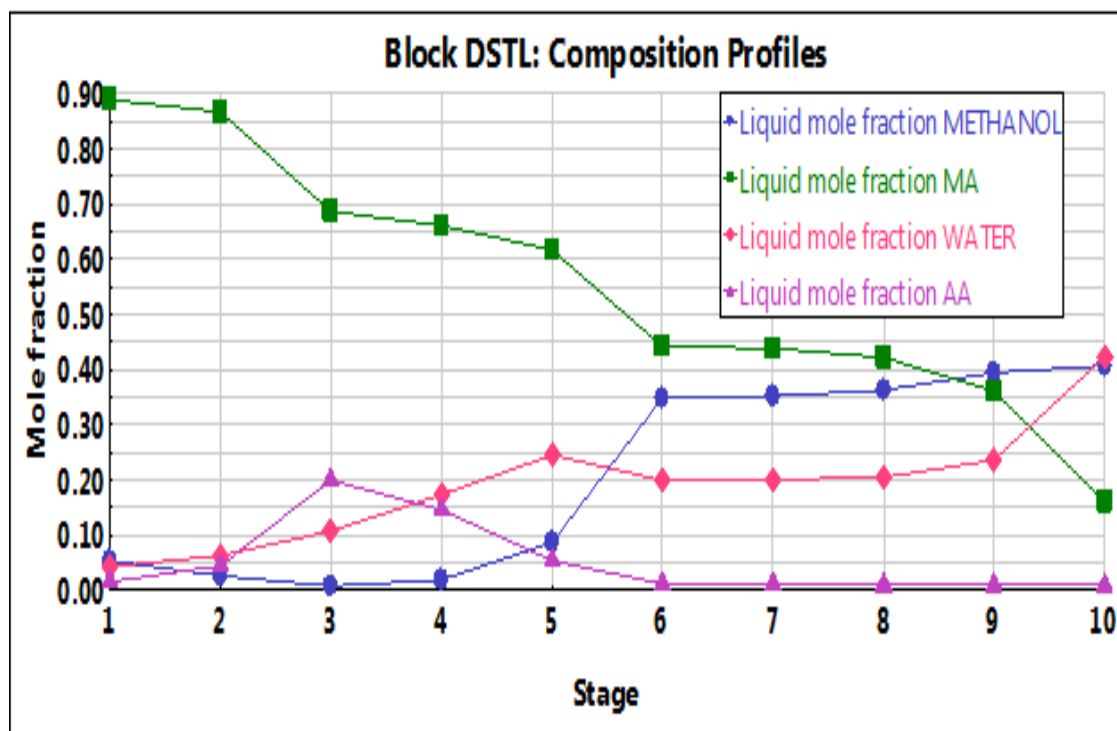


Fig.2 Composition profile of Methyl acetate in Aspen Plus

SIMULATION PURITY= 91%, EXPERIMENTAL PURITY= 93%

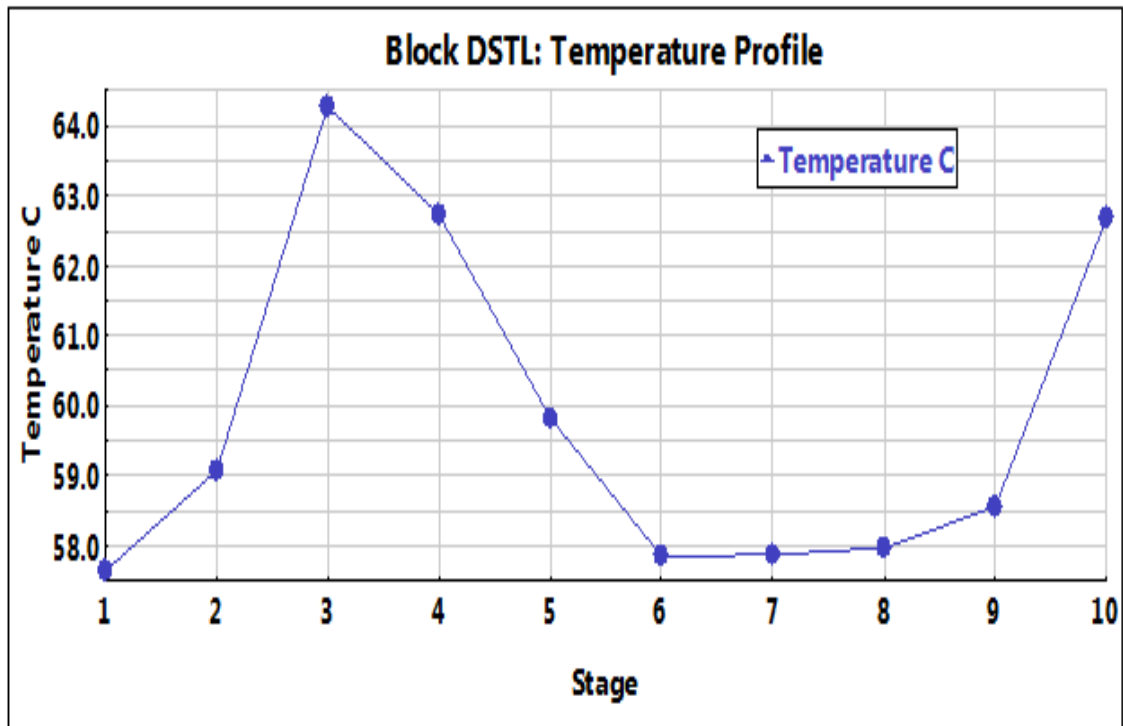
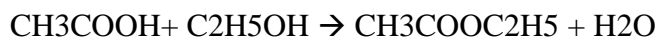


Fig.3 Temperature Plot in RD for methyl acetate synthesis

## 1. ETHYL ACETATE EXPERIMENTAL DETAIL

**Ethyl acetate** (systematically, ethyl ethanoate, commonly abbreviated EtOAc or EA) is the organic compound with the formula  $\text{CH}_3\text{-COO-CH}_2\text{-CH}_3$ . This colorless liquid has a characteristic sweet smell (similar to pear drops) and is used in glues, nail polish removers, decaffeinating tea and coffee, and cigarettes (see list of additives in cigarettes). Ethyl acetate is the ester of ethanol and acetic acid; it is manufactured on a large scale for use as a solvent.



$$r = m_{cat}(k_1 * x_{EA} * x_{H_2O} - k_2 * x_{AA} * x_{EtOH})$$

$$k_1 = k_1^0 \exp(-E_1/RT) = 0.147$$

$$k_2 = k_2^0 \exp(-E_2/RT) = 0.0268$$

$$E_1 = 49.3, E_2 = 66.2$$

$$K_1^0 = 4.24 \times 10^6$$

$$K_2^0 = 4.55 \times 10^8$$

Where

$m_{cat}$  is the mass of catalyst

T is temperature, K

R is universal gas constant = 8.314 J/gmmol<sup>0</sup>k

$E_1, E_2$  are the activation energy, Kjoule/mol

$k_1^0, k_2^0$  are the standard rate constant, mol / gm cat sec

**TABLE 3: OPERATING CONDITION FOR ETHYL ACETATE IN PILOT SCALE RD**

PARAMETERS	VALUE
PRESSURE	ATMOSPHERIC
REBOILER DUTY	1 KW
FEED 1 ( ETHANOL)	AT BOTTOM OF REACTIVE ZONE
FEED 2 (ACETIC ACID)	AT TOP OF REACTIVE ZONE
FEED 1 TEMPERATURE	70 C
FEED 2 TEMPERATURE	85 C
FEED 1 FLOW RATE	0.03 L/MIN
FEED 2 FLOW RATE	0.03 L/MIN
REFLUX RATE	0.25 l/min
DISTILLATE FLOW RATE	0.05 ml/min
REFLUX RATIO	5
INITIAL REBOILER HOLD UP	1 Ltr
MAXIMUM REBOILER CAPACITY	2 LTR
TOTAL SEGMENT	8
REBOILER	10 <sup>TH</sup> SEGMENT
CONDENSER TYPE	VERTICAL
FIRST TIME TO STEADY STATE	25 min
SECOND TIME TO STEADY STATE	55 min
FINAL TIME TO STEADY STATE	75 min
HEIGHT OF COLUMN	3 METER
PACKING IN REACTIVE ZONE	AMBERLYST 15 WET
PACKING IN RECTIFYING + STRIPPIG ZONE	KATAPAK S

**TABLE 4: EXPERIMENTAL TEMPERATURE DETAIL WITH TIME FOR ETHYL ACETATE**

TIME SEGMENT ↓(Temp) →	T1	T2	T3	T4	T5	T6	T7	T8	T9	REBOILER TEMP
5 min	32	34	37	38	39	38	35	35	35	65
10 min	32	34	37	37	38	35	36	34	33	65
15 min	65	35	36	37	38	36	36	34	35	64.5
20 min	69	70	80	38	38	35	36	31	35	65
25 min	71	72	82	82	81	74	75	77	77	65
30 min	71	72	82	84	80	75	76	76	79	65.5
35 min	72.5	72	82	84	81	75	76	77	77	65.5
40 min	72	74	80	83	80	74	75	76	80	67
45 min	72	73	81	83	79	75	78	75	79	68
50 min	73	75	80.5	82	80	76	76	76	78	68.5
55 min	74	76	81	82	79	75	76	77	80	69
60 min	74	76	81	81	79	75	75	77	80	70
65 min	75	77	80	82	77	77	75	76	82	72
70 min	75	79	81	81	78	76	76	76	81	72
75 min	74	79	80	80	76	75	76	77	81	72
80 min	75	79	80.5	81	77	75	76	76	81	72
85 min	75	78	80	81	77	76	76	76	80	72.5
90 min	75	79	80	81	77	76	76	75	80	72.5

ETHYL ACETATE SIMULATION IN ASPEN PLUS: OPERATING CONDITIONS ARE SAME AS OF EXPERIMENT AS DETAILED IN TABLE 1

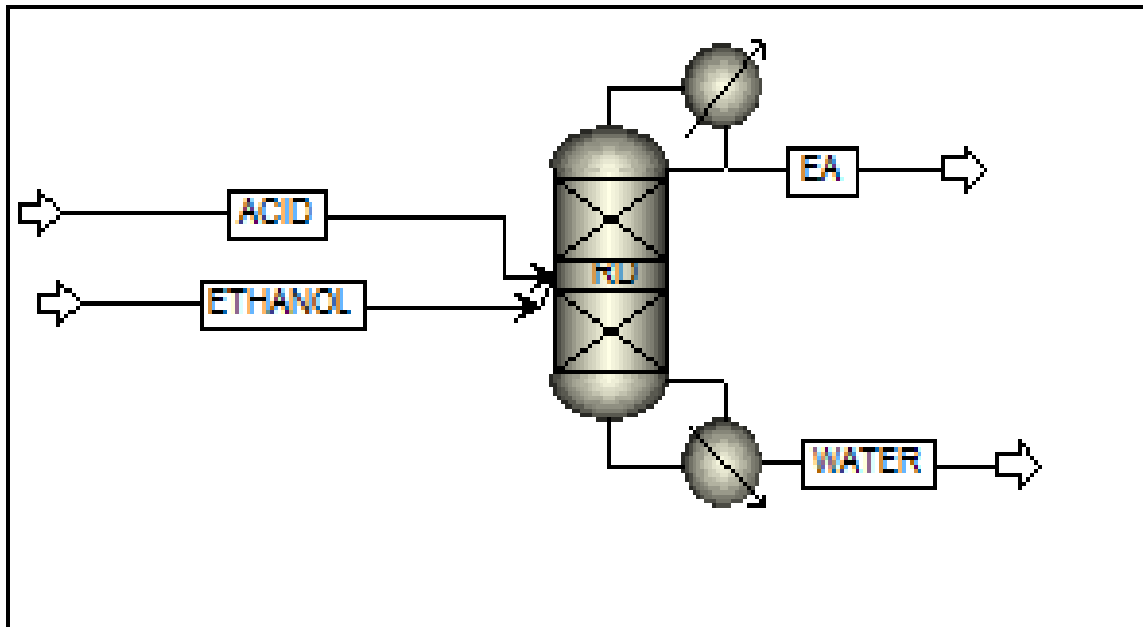


Fig 4. Schematic of ethyl acetate synthesis in aspen plus

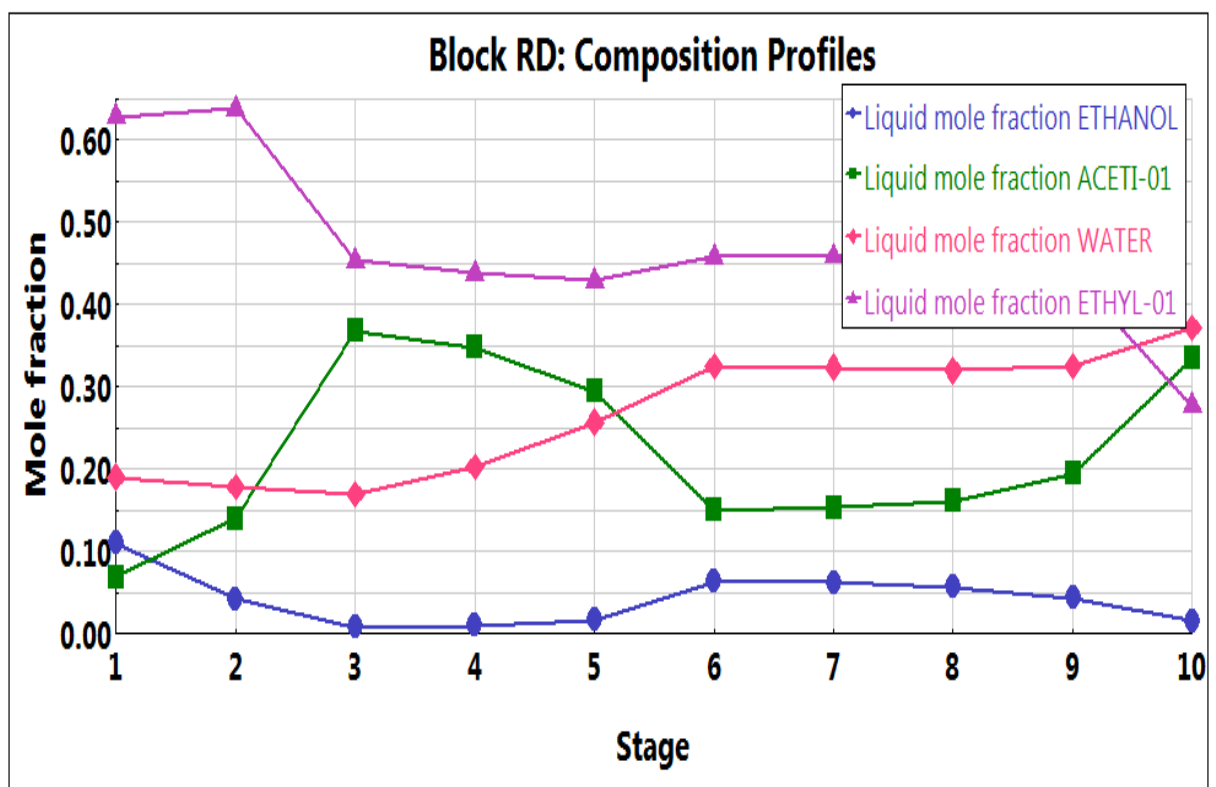


Fig. 5 Composition Profile for ethyl acetate  
SIMULATION PURITY=62%, EXPERIMENTAL PURITY=70%



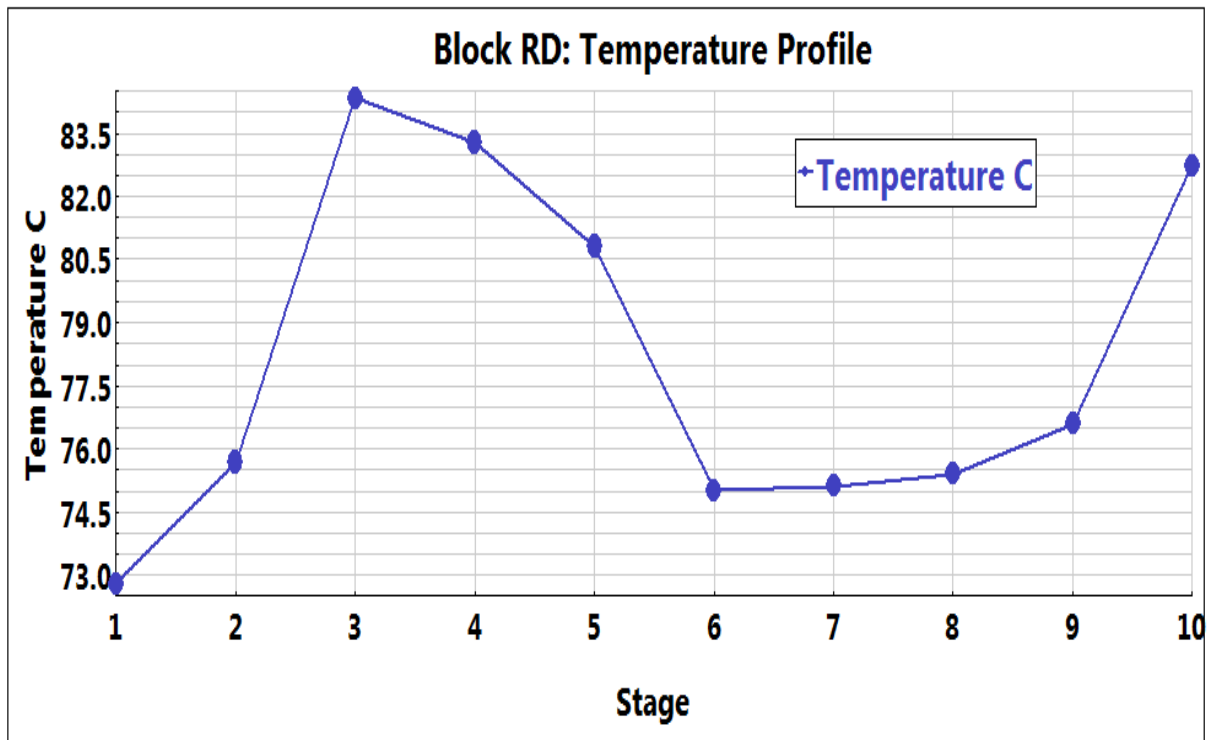
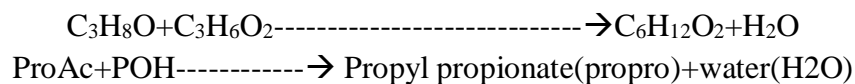


Fig. 6 Temperature profile for ethyl acetate

## 2. PROPYL ACETATE:

**Propyl acetate**, also known as **propyl ethanoate**, is a chemical compound used as a solvent. This clear, colorless liquid is known by its characteristic odor of pears. Due to this fact, it is commonly used in fragrances and as a flavor additive. It is formed by the esterification of acetic acid and 1-propanol, often via Fischer–Speier esterification.

Heterogeneous catalyzed esterification of propionic acid (ProAc) with propanol(POH) to propyl-propionate and water can be represented as:



At any time rate of formation of propyl propionate is given by when homogeneous catalyst is used:

$$r_{\text{proprio}} = K_1 C_{\text{POH}} C_{\text{ProAc}} - K_{-1} C_{\text{proprio}} C_{\text{H}_2\text{O}}$$

When the rate of reaction of propyl propionate is zero it means that equilibrium is attained, and rate of formation is equal to rate of disappearance.

$$K_1 C_{\text{POH}} C_{\text{ProAc}} = K_{-1} C_{\text{proprio}} C_{\text{H}_2\text{O}}$$

$$K_{\text{eq}} = K_1 / K_{-1} = C_{\text{proprio}} C_{\text{H}_2\text{O}} / C_{\text{POH}} C_{\text{ProAc}}$$

When heterogeneous catalyst is used the rate is affected by the amount of catalyst used.

Rate equation in terms of forward rate constant and equilibrium constant can be written as:

$$r_i = (m_{\text{catdry}} * v_i) \left( K_1(T) C_{\text{Proac}} C_{\text{POH}} - \frac{K_1(T) C_{\text{proprio}} C_{\text{H}_2\text{O}}}{K_{\text{eq}}(T)} \right)$$

$$K_1(T) = 7.381 * 10^7 \exp \left( -5.963 * \frac{10^4}{RT} \right)$$

$$K_{eq} = 6.263 \exp\left(\frac{4.519 * 10^3}{RT}\right)$$

$C_{Proac}$  = Concentration of propionic acid

$C_{POH}$  = Concentration of propanols

$C_{propro}$  = Concentration of propyl propionate

$C_{H_2O}$  = Concentration of water

$r_i$  = rate of reaction

$m_{catdry}$  = mass of dry catalyst used (500gms in our case)

$K_1$  = forward rate constant

$K_{eq}$  = equilibrium rate constant for the reaction

$R$  = universal rate constant

$T$  = temperature

$v_i$  = stoichiometric coefficient of component  $i$ . (where  $i=1 \dots N_c$ )

$N_c$  = total number of component.

**TABLE 5: OPERATING CONDITION FOR PROPYL ACETATE**

PARAMETERS	VALUE
PRESSURE	ATMOSPHERIC
REBOILER DUTY	2 KW
FEED 1 ( PROPANOL)	AT BOTTOM OF REACTIVE ZONE
FEED 2 (ACETIC ACID)	AT TOP OF REACTIVE ZONE
FEED 1 TEMPERATURE	85 C
FEED 2 TEMPERATURE	90 C
FEED 1 FLOW RATE	0.03 L/MIN
FEED 2 FLOW RATE	0.03 L/MIN
REFLUX RATE	0.25 l/min
DISTILLATE FLOW RATE	0.05 ml/min
REFLUX RATIO	5
INITIAL REBOILER HOLD UP	1 Ltr
MAXIMUM REBOILER CAPACITY	2 LTR
TOTAL SEGMENT	8
RECTIFYING SECTION	1-3
REACTIVE ZONE	3-6
STRIPPING SECTION	6-9
REBOILER	10 <sup>TH</sup> SEGMENT
CONDENSER TYPE	VERTICAL
HEIGHT OF COLUMN	3 METER
PACKING IN REACTIVE ZONE	AMBERLYST 15 WET
PACKING IN RECTIFYING + STRIPPING ZONE	KATAPAK S

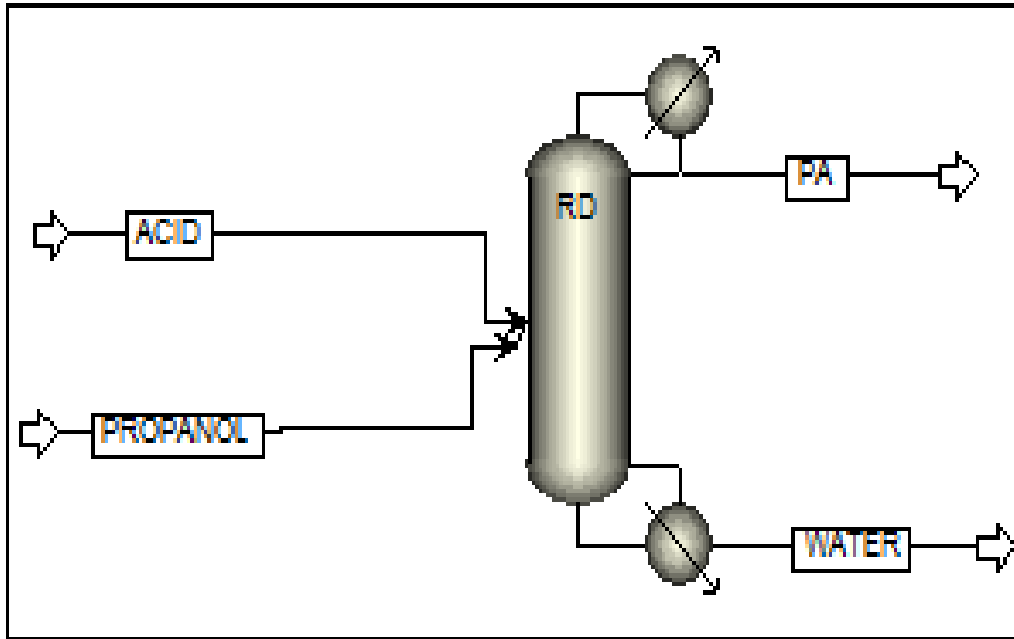


Fig. 7 Schematic for propyl acetate

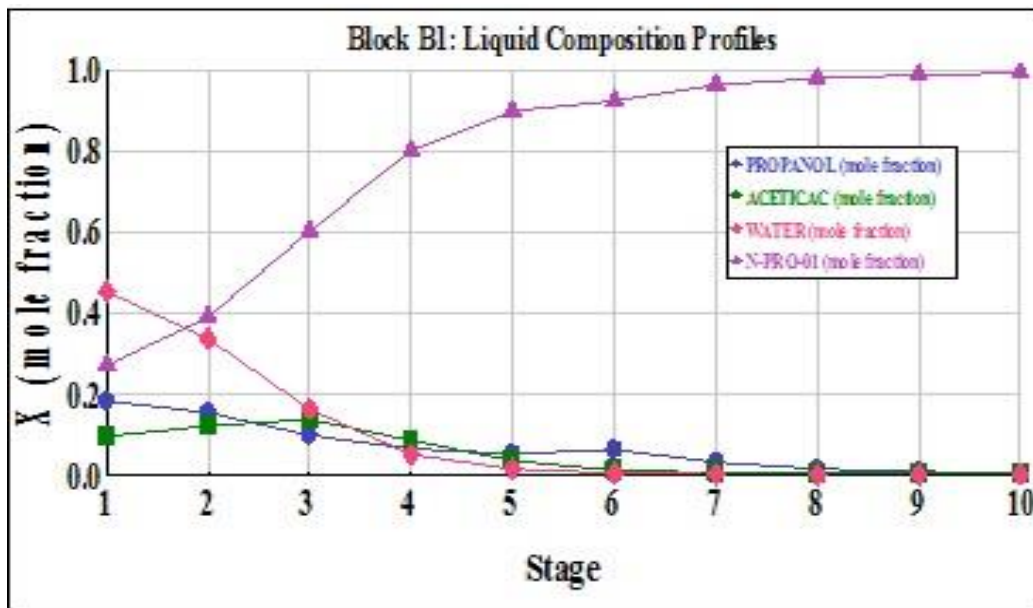


Fig. 8 Composition Plot for propyl acetate

SIMULATION PURITY= 97%

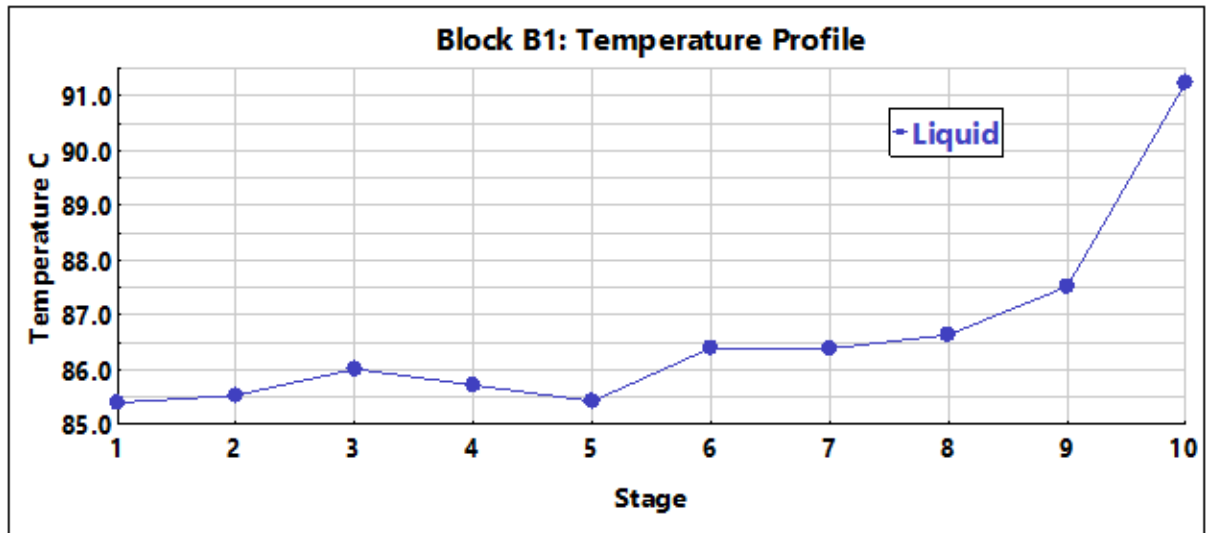
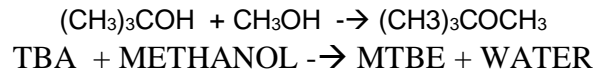


Fig. 9 Temperature plot for propyl acetate

### 3. METHYL TERT BUTYL ETHER

**Methyl tert-butyl ether** (also known as **MTBE**, **tert-butyl methyl ether**, **tertiary butyl methyl ether** and **tBME**) is an organic compound with molecular formula  $(CH_3)_3COCH_3$ . MTBE is a volatile, flammable, and colorless liquid that is sparingly soluble<sup>[1]</sup> in water. It has a minty odor vaguely reminiscent of diethyl ether, leading to unpleasant taste and odor in water. MTBE is a gasoline additive, used as an oxygenate to raise the octane number. Its use is controversial in the US and declining in use in part because of its occurrence in groundwater and legislation favoring ethanol.



$$r = m_{cat}(k_1 * x_{MTBE} * x_{H_2O})$$

$$k_1 = k_1^0 \exp(-E_1/RT)$$

$$E_1 = 130.4$$

$$K_1^0 = 6.028 \times 10^{19}$$

Where

$m_{cat}$  is the mass of catalyst

T is temperature, K

R is universal gas constant = 8.314 J/gmmol<sup>0</sup>k

$E_1$  is the activation energy, Kjoule/mol

$k_1^0$ , is the standard rate constant, l/mol min

**TABLE 6: OPERATING CONDITION FOR MTBE**

PARAMETERS	VALUE
PRESSURE	ATMOSPHERIC
REBOILER DUTY	2 KW
FEED 1 ( METHANOL)	AT BOTTOM OF REACTIVE ZONE
FEED 2 (TBA)	AT TOP OF REACTIVE ZONE
FEED 1 TEMPERATURE	60 C
FEED 2 TEMPERATURE	75 C
FEED 1 FLOW RATE	0.02 L/MIN
FEED 2 FLOW RATE	0.02 L/MIN
REFLUX RATE	0.25 l/min
DISTILLATE FLOW RATE	0.05 ml/min
REFLUX RATIO	5
INITIAL REBOILER HOLD UP	1 Ltr
MAXIMUM REBOILER CAPACITY	2 LTR
TOTAL SEGMENT	8
REBOILER	10 <sup>TH</sup> SEGMENT
CONDENSER TYPE	VERTICAL
FIRST TIME TO STEADY STATE	20 min
SECOND TIME TO STEADY STATE	50 min
FINAL TIME TO STEADY STATE	75 min
HEIGHT OF COLUMN	3 METER
PACKING IN REACTIVE ZONE	AMBERLYST 15 WET
PACKING IN RECTIFYING + STRIPPING ZONE	KATAPAK S

**TABLE 7: EXPERIMENTAL TEMPERATURE DATA FOR MTBE**

TIME SEGMENT ↓(Temp) →	T1	T2	T3	T4	T5	T6	T7	T8	T9	REBOILER TEMP
5 min	32	34	37	38	39	38	35	35	35	65
10 min	32	34	37	37	38	35	36	34	33	65
15 min	65	35	36	37	38	36	36	34	35	64.5
20 min	55	55	54	52	55	34	33	34	35	65
25 min	55	54	55	53	55	53	31	33	35	65
30 min	56	57	55	56	55	53	31	32	33	65.5
35 min	55	56	54	56	58	54	48	45	40	65.5
40 min	60	58	53	55	58	57	51	52	51	67
45 min	65	61	63	66	69	66	65	59	57	68
50 min	54	54	55	59	60	54	56	56	58	68.5
55 min	55	56	51	52	59	55	56	57	50	69
60 min	54	56	51	51	59	55	55	57	50	67
65 min	55	57	50	52	57	57	55	56	52	65
70 min	55	59	51	51	58	56	56	56	51	65
75 min	54	59	50	50	56	55	56	57	51	65.8
80 min	55	59	50	51	57	55	56	56	51	72
85 min	55	58	50	51	57	56	56	56	50	71
90 min	55	59	50	51	57	56	56	55	50	71

ETHYL ACETATE SIMULATION IN ASPEN PLUS: OPERATING CONDITIONS ARE SAME AS OF EXPERIMENT AS DETAILED IN TABLE 6

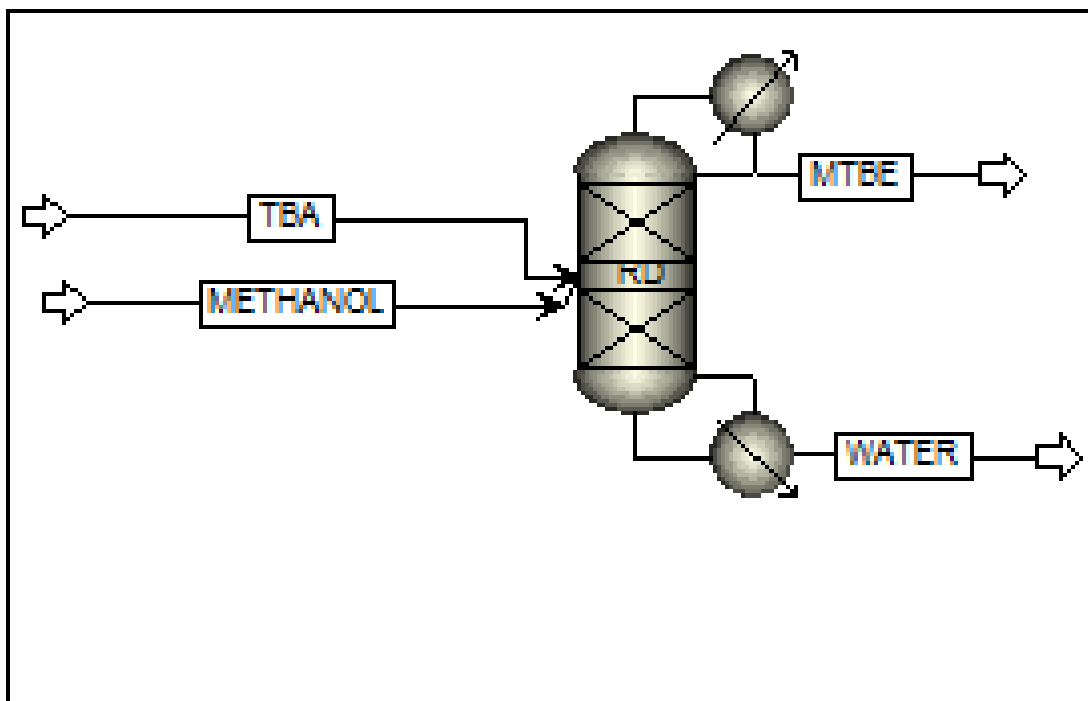


Fig 10 : Schematic for MTBE synthesis

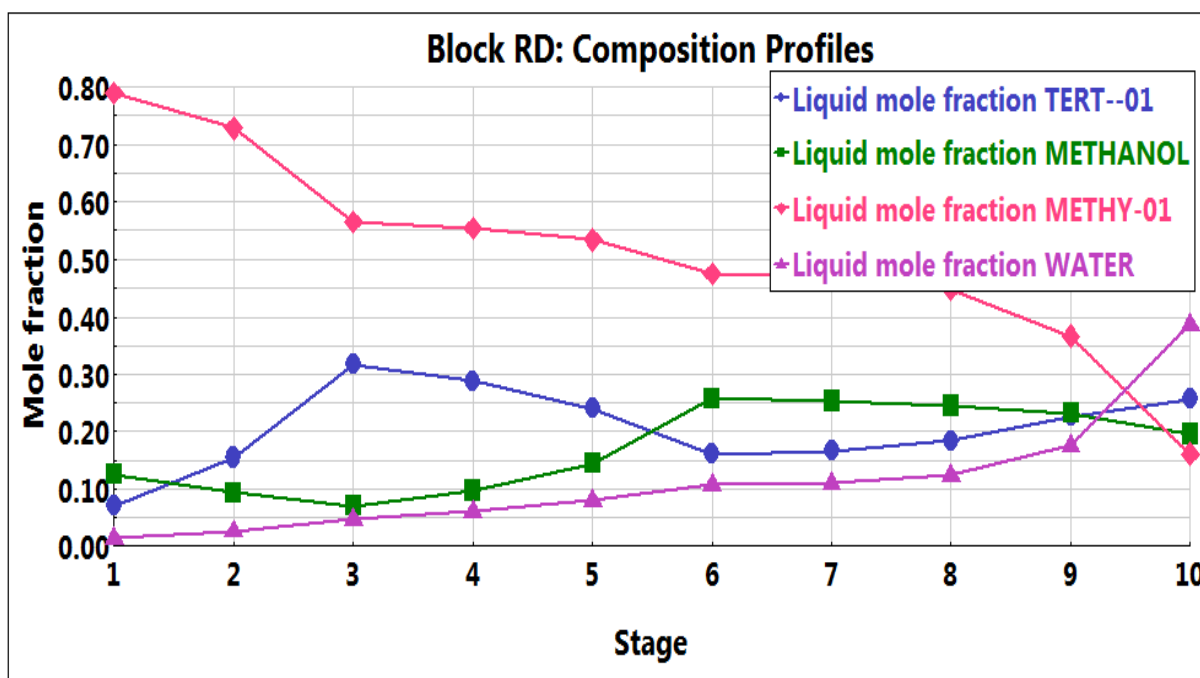


Fig. 11: Composition plot for MTBE

Purity= 80%, EXPERIMENTAL PURITY= 85%

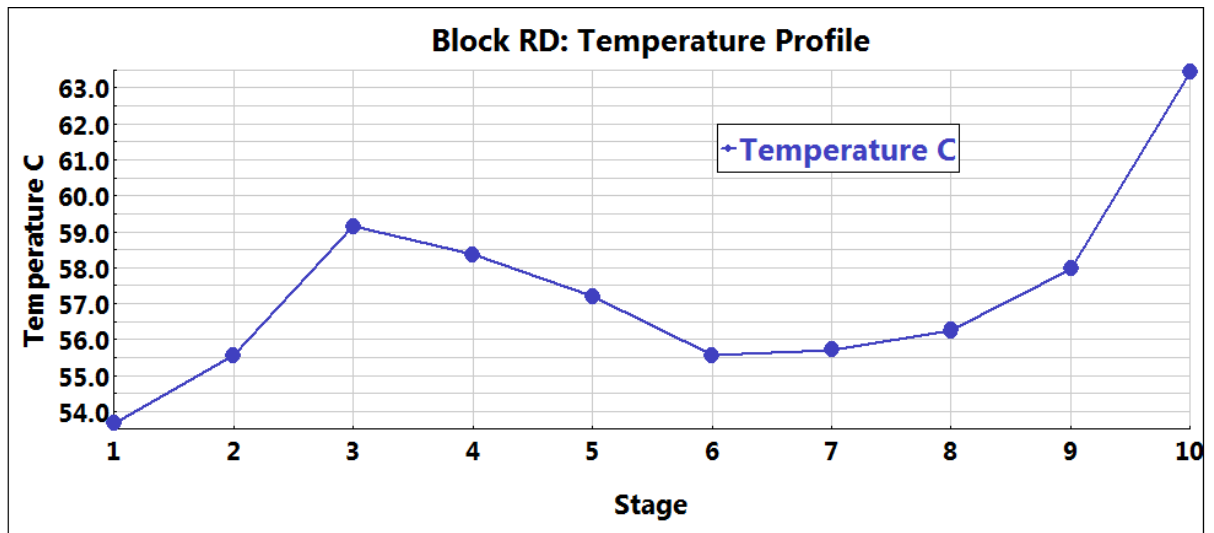


Fig. 11 Temperature Plot for MTBE

#### 4. ETBE Synthesis in Pilot RD

**Ethyl *tert*-butyl ether (ETBE)** is commonly used as an oxygenate gasoline additive in the production of gasoline from crude oil. ETBE offers equal or greater air quality benefits than ethanol, while being technically and logistically less challenging. Unlike ethanol, ETBE does not induce evaporation of gasoline, which is one of the causes of smog, and does not absorb moisture from the atmosphere.

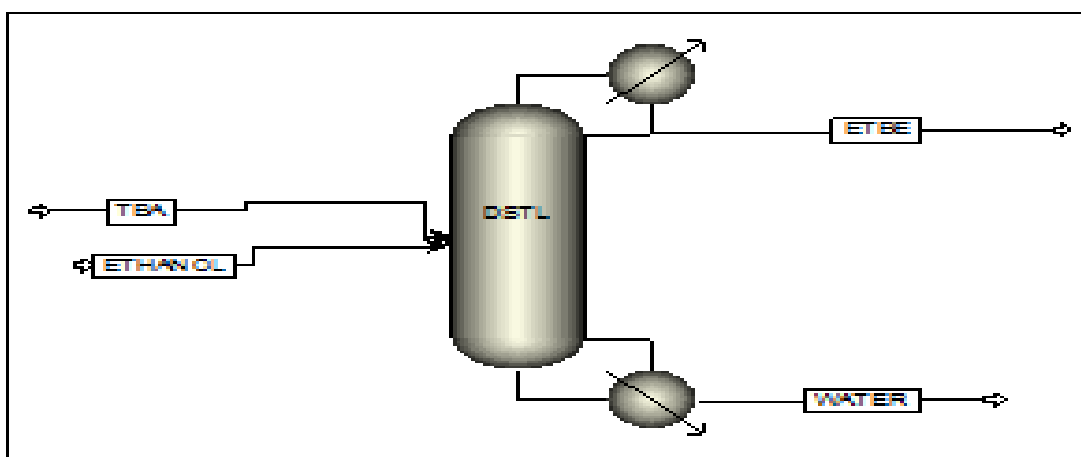
**TABLE 8: Operating Condition for ETBE**

PARAMETERS	VALUE
PRESSURE	ATMOSPHERIC
REBOILER DUTY	2 KW
FEED 1 ( METHANOL)	AT BOTTOM OF REACTIVE ZONE
FEED 2 (TBA)	AT TOP OF REACTIVE ZONE
FEED 1 TEMPERATURE	60 C
FEED 2 TEMPERATURE	75 C
FEED 1 FLOW RATE	0.02 L/MIN
FEED 2 FLOW RATE	0.02 L/MIN
REFLUX RATE	0.25 l/min
DISTILLATE FLOW RATE	0.05 ml/min
REFLUX RATIO	5
INITIAL REBOILER HOLD UP	1 Ltr
MAXIMUM REBOILER CAPACITY	2 LTR
TOTAL SEGMENT	8
RECTIFYING SECTION	1-3
REACTIVE ZONE	3-6
STRIPPING SECTION	6-9
REBOILER	10 <sup>TH</sup> SEGMENT
CONDENSER TYPE	VERTICAL
FIRST TIME TO STEADY STATE	30 min
FINAL TIME TO STEADY STATE	70 min
HEIGHT OF COLUMN	3 METER
PACKING IN REACTIVE ZONE	AMBERLYST 15 WET
PACKING IN RECTIFYING + STRIPPING ZONE	KATAPAK S

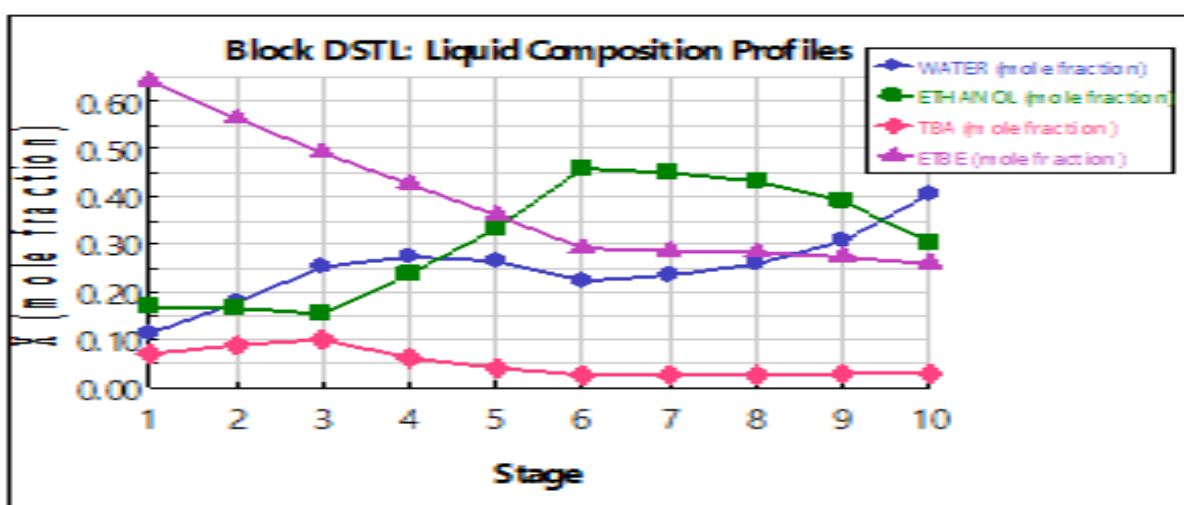
**TABLE 9: EXPERIMENTAL TEMPERATURE DATA FOR ETBE**

TIME SEGMENT→	T1	T2	T3	T4	T5	T6	T7	T8	T9	Reboiler
10	32	36	32	37	37	35	34	30	31	61
20	62	63	60	38	38	35	35	31	32	63
30	61	64	60	66	67	62	56	55	54	63
40	64	64	62	66	77	62	56	49	55	65
50	65	68	64	70	75	66	57	53	54	65
60	65	68	63	67	73	66	58	52	53	66
70	66	66	63	67	76	65	59	57	53	65
80	67	66	64	68	70	63	54	53	52	67
90	65	69	63	65	67	63	55	52	53	67
100	65	69	63	65	67	63	55	52	52	67

**ETBE SIMULATION IN ASPEN PLUS: OPERATING CONDITIONS ARE SAME AS OF EXPERIMENT AS DETAILED IN TABLE 8**



**Fig. 12 Schematic for ETBE Production**



**Fig 13 Composition plot for ETBE**



Purity= 66 %, EXPERIMENTAL PURITY= 70%

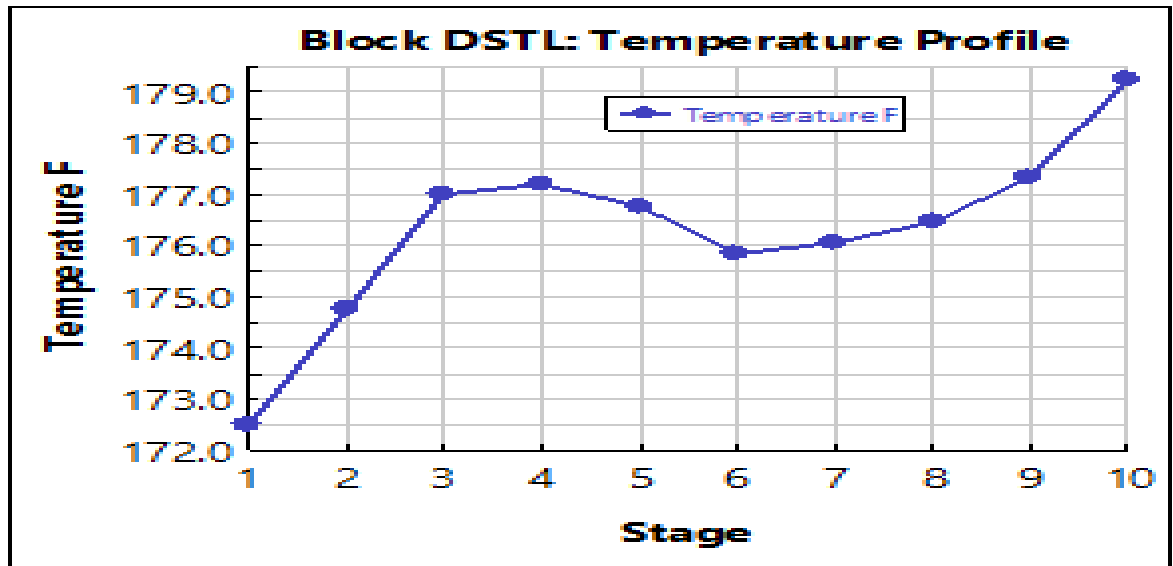
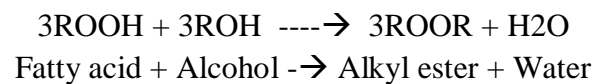


Fig. 14 Temperature Plot for ETBE

## 5. BIODIESEL SYNTHESIS PROCESS:

Transesterification is the chemical process of converting one ester, in this case the glycerol esters that constitute vegetable oils, into another ester such as the alkyl monoesters that compose biodiesel. This process occurs by reacting the vegetable oil with alcohol in the presence of an alkaline or acidic catalyst as per the following reaction:



$$r = m_{\text{cat}}(k_1 * x_{\text{BD}} * x_{\text{H}_2\text{O}} - k_2 * x_{\text{FA}} * x_{\text{EtOH}})$$

$$k_1 = k_1^0 \exp(-E_1/RT) = 3.4 \times 10^{10}$$

$$k_2 = k_2^0 \exp(-E_2/RT) = 8.3 \times 10^{10}$$

$$E_1 = 13.14, E_2 = 6.20$$

Where

$m_{\text{cat}}$  is the mass of catalyst

T is temperature, K

R is universal gas constant = 8.314 J/gmmol<sup>0</sup>k

$E_1, E_2$  are the activation energy, Kcal/mol

$k_1^0, k_2^0$  are the standard rate constant, Lmole/sec

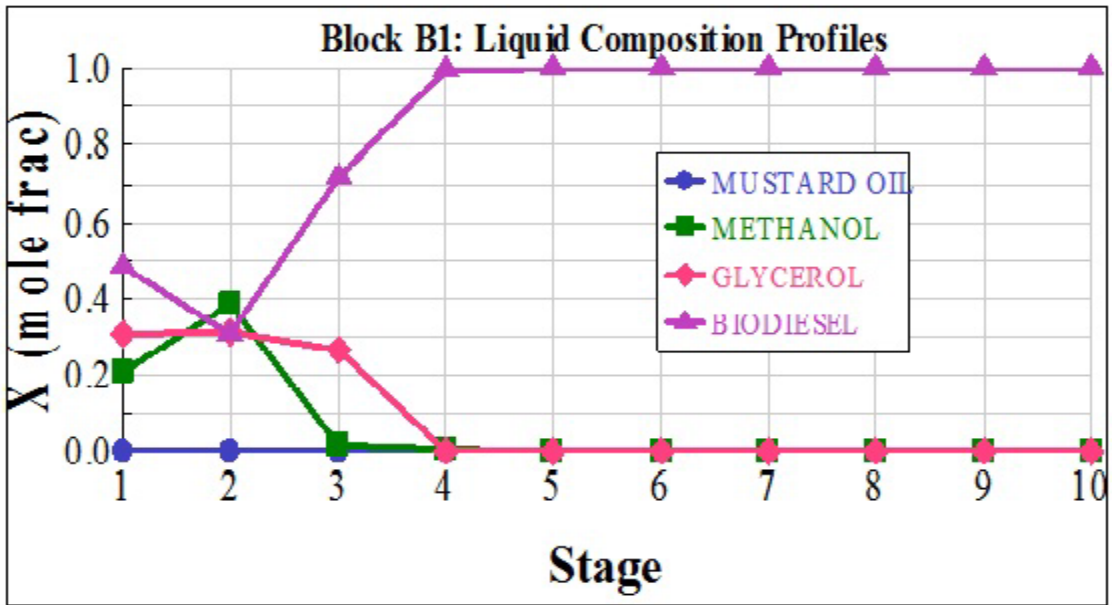


Fig. 15 Composition plot for biodiesel

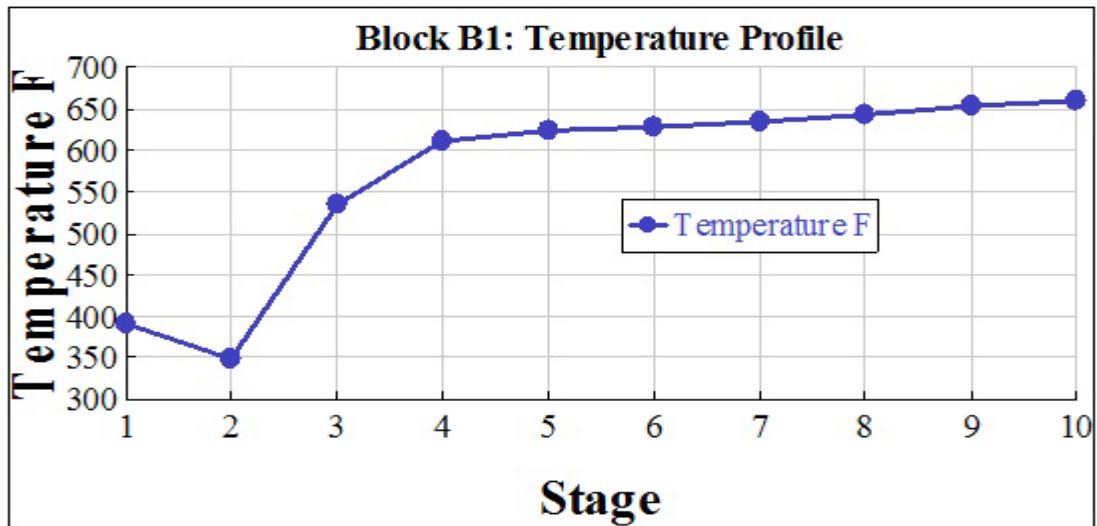


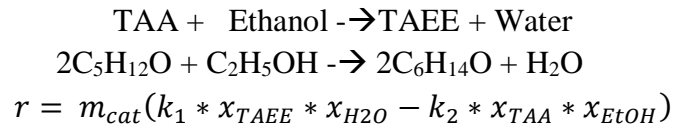
Fig. 16 Temperature profile for biodiesel



Fig. 17 Biodiesel

6. **TAAE SYNTHESIS:** It stands for tertiary amyl ethyl ether. It is excellent blending component due to its low volatility, high octane number and they do not contain aromatics and olefins. It is formed by etherification reaction of tert amyl alcohol and ethanol in presence of acidic catalyst which may be either homogeneous or heterogeneous in nature.

The chemical reaction and kinetic is shown below:



Where

$m_{\text{cat}}$  is the mass of catalyst

$k_1 = \exp(15.189 - 6597.3/T)$ ,

$k_2 = \exp(14.490 - 6372.9/T)$

T is temperature

$k_1$  is forward rate constant, kgmole/sec

$k_2$  is backward rate constant, kgmole/sec

x is concentration of components

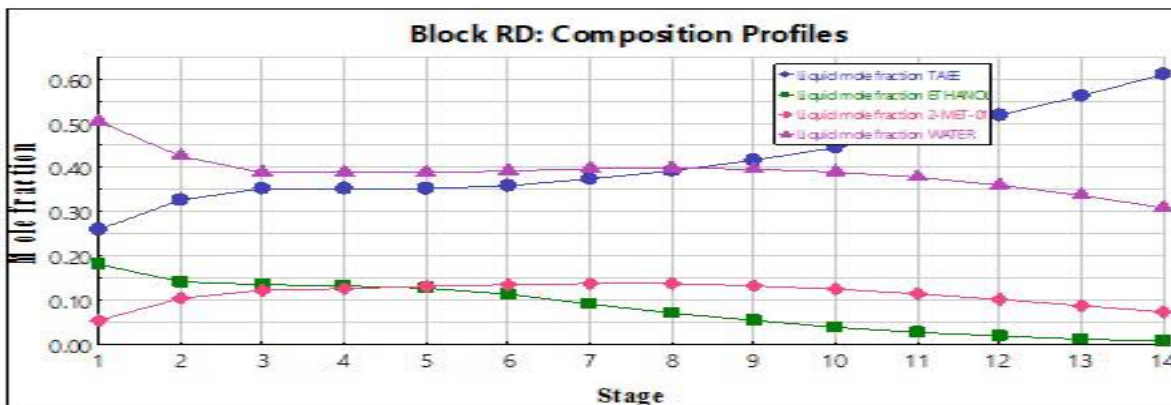


Fig. 17 Composition profile for TAAE synthesis

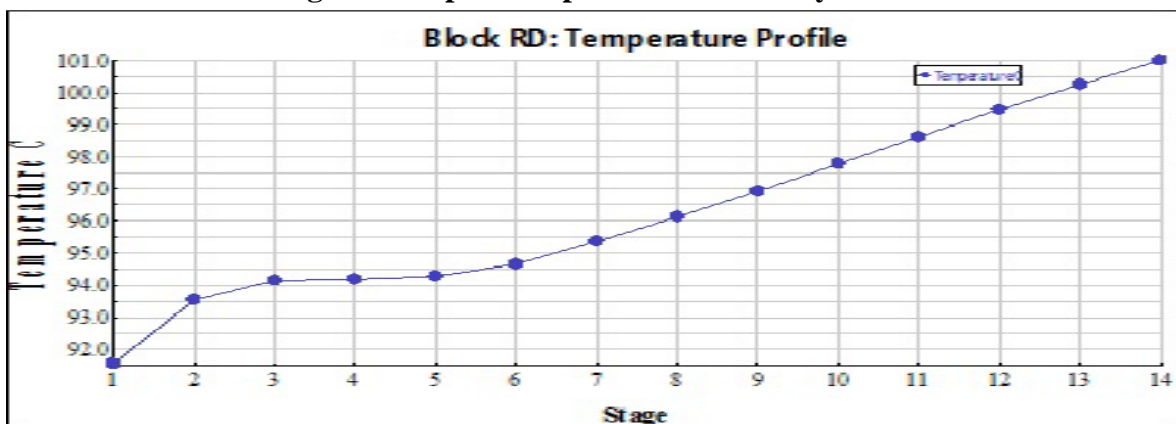


Fig. 18 Temperature profile for TAAE