Process Development on Aspen plus

Under the guidance of Dr Sumit Kamal

Design Credit Course

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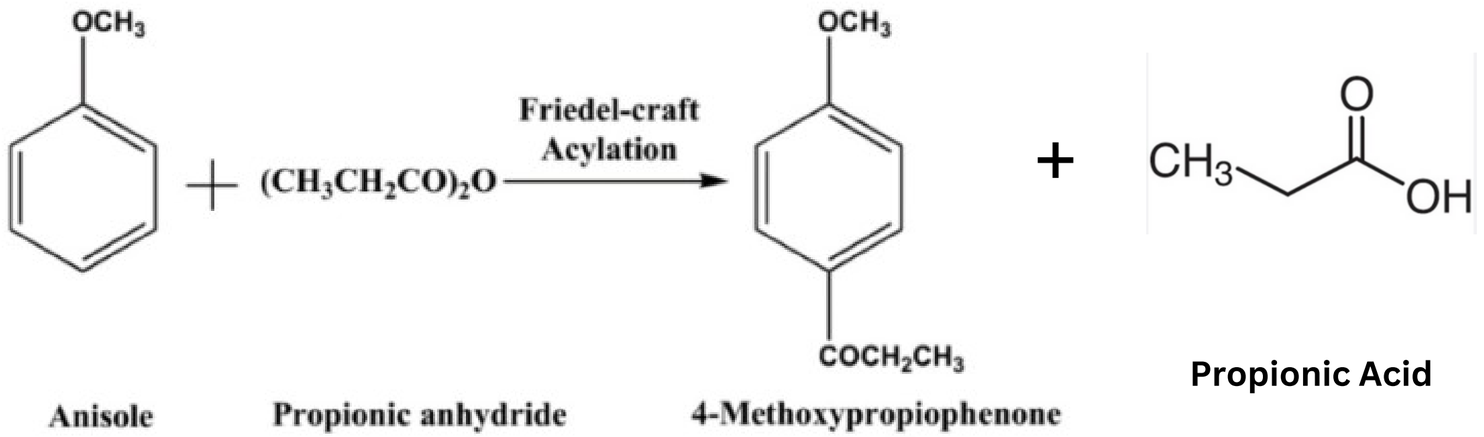
Friedel Craft Acylation reaction of Anisole with Propionic anhydride



Anisole | Propionic anhydride | 4-Methoxypropiophenone | Propionic Acid

4- Methoxypropiophenone are usually prepared by the acylation of anisole with propionyl chloride using AlCl3 as catalyst.

Importance of Methoxypropiophenone:

- 4-Methoxypropiophenone is an intermediate for the production of anethole, which is widely used in preparation of perfumes and flavors.
- Methoxypropiophenone are found to have wide applications in the area of fine chemical synthesis.

There are two steps involved in the production of 4-Methoxypropiophenone

1. The main reaction and formation of reaction mixture of reactant and product.

Batch Reactor

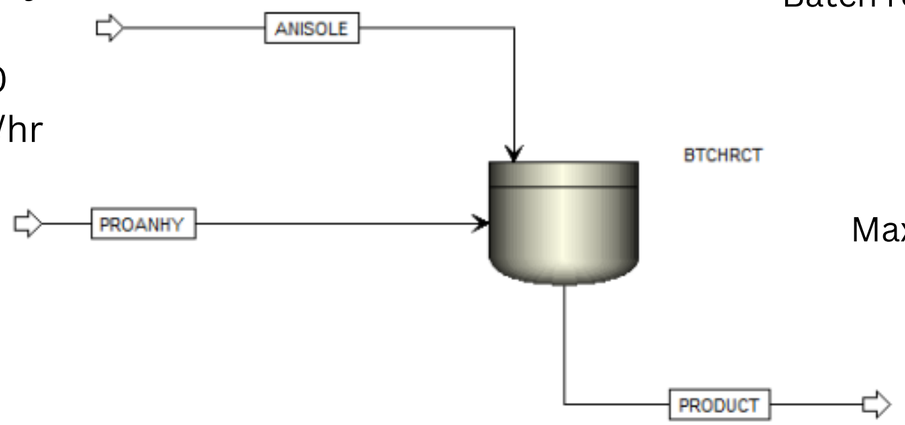
2. Separation of each components by distillation for further use.

Batch Distillation

Batch Reaction

- Anisole is fed in continuously and propionic anhydride is fed once into the reactor.
- Anisole and propionic anhydride are partially converted into 4-Methoxypropiophenone and propionic acid.
- Reaction is carried out in a batch reactor to form 4-Methoxypropiophenone and propionic acid along with unreacted Anisole and propionic anhydride.

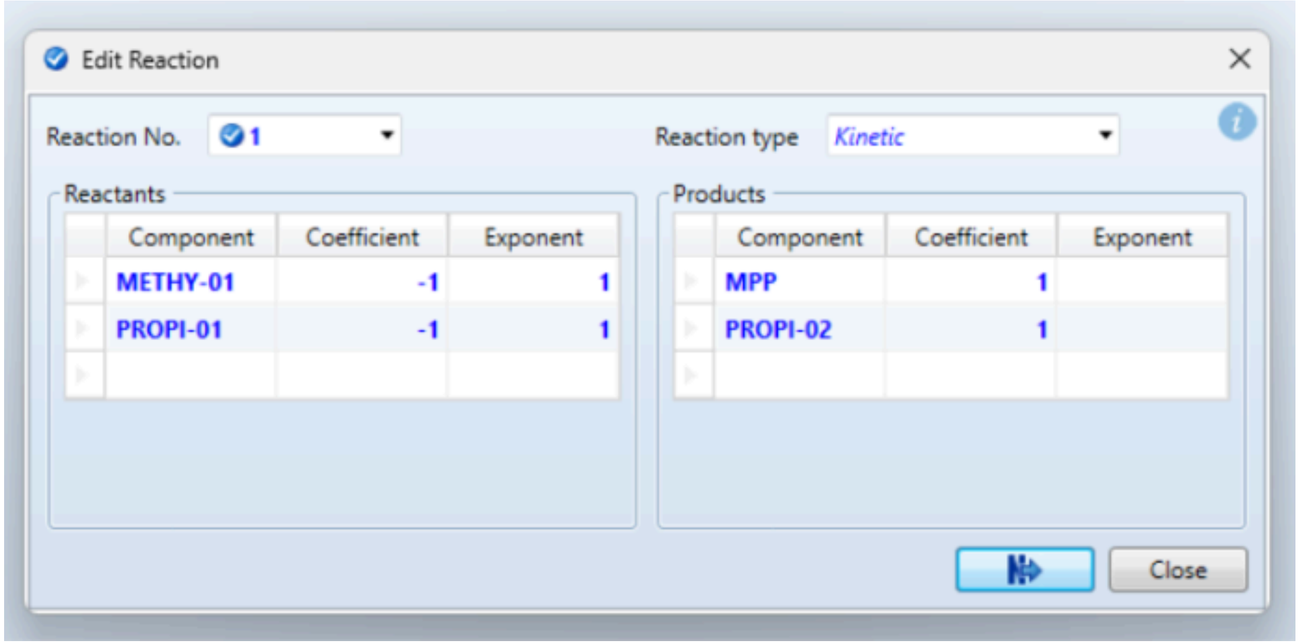
Anisole and Propionic Anhydride.
Pressure: 1 bar
Vapor Fraction: 0
Flow rate: 10 Kmol/hr



Batch reactor conditions and specifications:
Temperature: 75 deg Celsius
Reactor pressure: 1 atm
Catalyst loading: 0.5 Kg
Batch feed time: 1 hour
Maximum calculation time: 1.5 Hour
Stop Value: 1.5 Hour

Method : NRTL RK METHOD

Reaction Kinetics



Reaction type: Kinetic
Reaction: Anisole + Propionic Anhydride → 4-Methoxypropiophenone + Propionic Acid
Reacting phase: Liquid
Kinetic factor = K T^n exp(-E/RT), K = 7.098 x 10^ -5 , n = 0, E=11450 J/kmol

Results and Observations

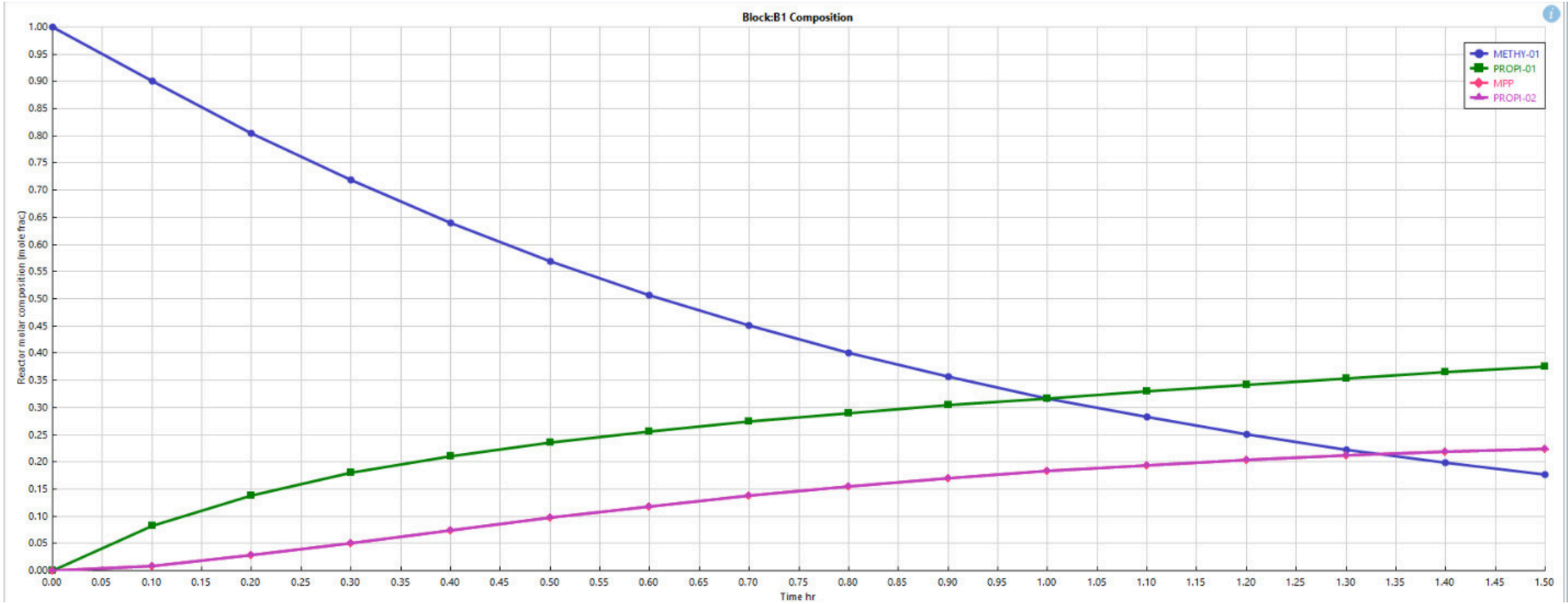
Presentations are communication tools that can be used as demonstrations, lectures, speeches, reports, and more. It is mostly presented before an audience. It serves a variety of purposes, making presentations powerful tools for convincing and teaching.

- Block calculations were completed normally.
- Property calculations were completed normally

	Units	ANISOLE	PROANHY	PRODUCT
− Mole Flows	**kmol/hr**	**10**	**10**	**16.6667**
METHY-01	kmol/hr	10	0	2.93328
PROPI-01	kmol/hr	0	10	6.26662
MPP	kmol/hr	0	0	3.73338
PROPI-02	kmol/hr	0	0	3.73338
− Mole Fractions				
METHY-01		1	0	0.175997
PROPI-01		0	1	0.375997
MPP		0	0	0.224003
PROPI-02		0	0	0.224003
− Mass Flows	**kg/hr**	**1081.4**	**1301.44**	**2022.37**
METHY-01	kg/hr	1081.4	0	317.205
PROPI-01	kg/hr	0	1301.44	815.56
MPP	kg/hr	0	0	613.037
PROPI-02	kg/hr	0	0	276.567
− Mass Fractions				
METHY-01		1	0	0.156848
PROPI-01		0	1	0.40327
MPP		0	0	0.303128
PROPI-02		0	0	0.136754
Volume Flow	l/min	20.8799	25.5971	33.6442

Conversion: 37.33%

- As Anisole is batch feed, its composition is continuously decreasing with time.
- The composition of 4- MPP and propionic acid is increasing as conversion in changing.
- Propionic anhydride composition is increasing as it is in continuous feed.



Batch Distillation

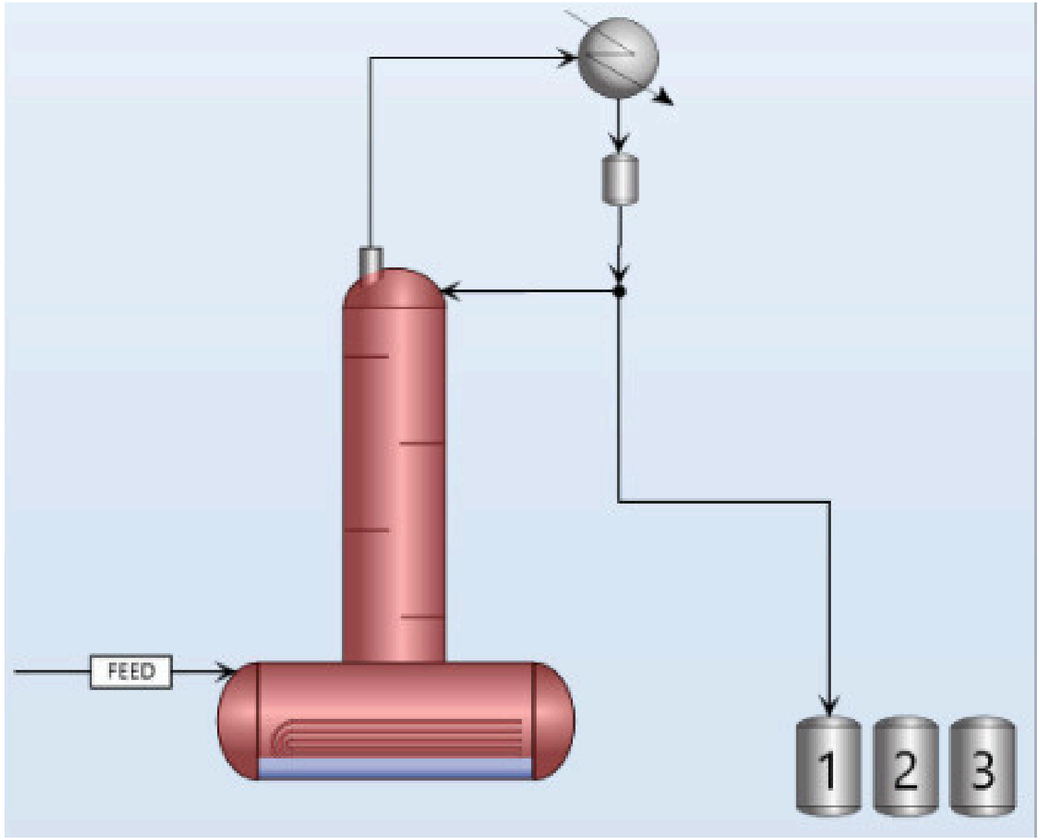
Batch distillation refers to the process of separating the components of a liquid mixture in batches. The distillation reactor is again charged with more mixture and the process is repeated.

Batch distillation on Aspen Plus:

We have a reaction mixture of 4 components that is Anisole, propionic anhydride, 4-Methoxypropiophenone and propionic acid which we now want to separate using batch distillation.

Boiling points are:

- Anisole: 154 deg Celcius
- Propionic Anhydride: 167 deg Celcius
- 4-Methoxypropiophenone: 243deg Celcius
- propionic acid: 141 deg Celcius.



Method : UNIFAC

Feed conditions are:

- Feed contains the reaction mixture.
- Temperature: 25 deg Celcius
- Pressure: 1 atm
- Total Flow rate: 10 kg/min
- Mass Fraction of each component is: 0.25

Batch conditions and specifications:

- Number of stages: 25
- Number of receiver: 3
- Initial condition: Total reflux
- Condenser pressure: 15 atm
- Column Pressure Drop: 0.0986923 atm
- Stage holdup: 0.005 Kg
- Condenser: Total
- Geometry specification of reactor: Horizontal
- Volume: 10L
- Diameter: 20 cm
- Heat transfer specific duty: 1.4 kW
- Total initial charge: 8 Kg

Column internals

- Internal Type: Trayed
- Tray spacing 14.5 cm
- Diameter: 10 cm

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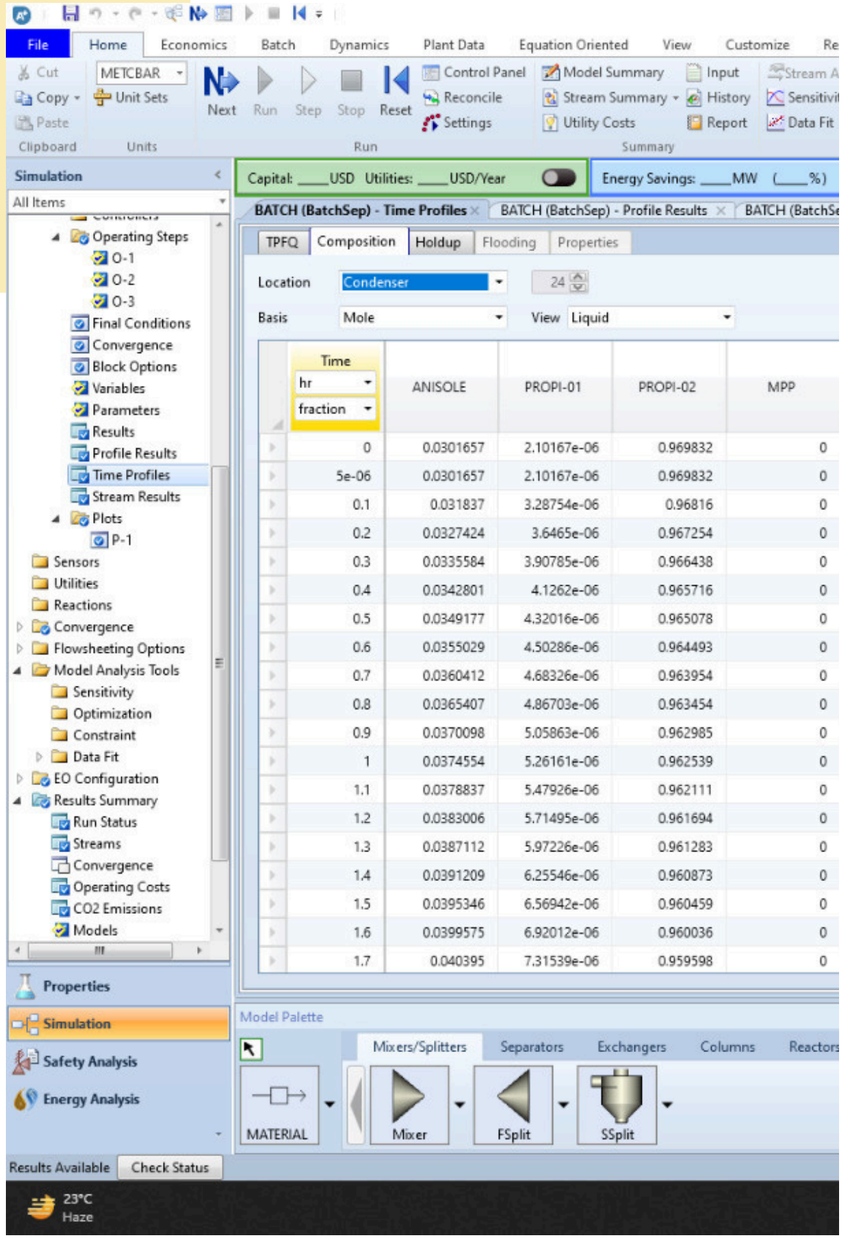
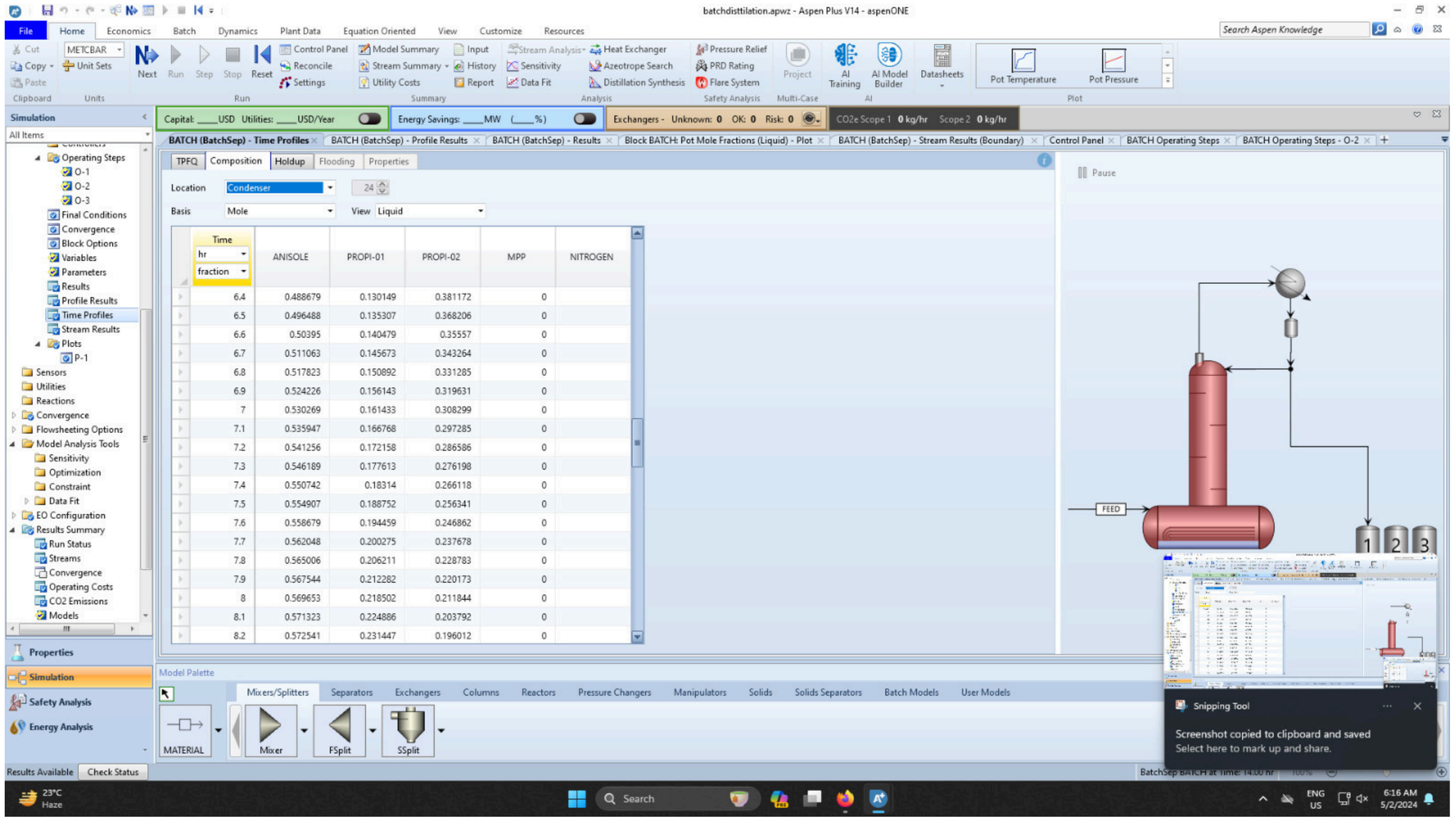


Operating steps:

- Reflux ratio: 40
- Total duration of reaction: 14 Hours
- Duration of 1st liquid distillate receiver: 4.5 hours
- Duration of 2nd liquid distillate receiver: 6 hours
- Duration of 3rd liquid distillate receiver: 3.5 hours

- Propionic Acid is the most volatile among the four as it has the lowest boiling point so firstly it will vaporize and will be collected in the first distillate liquid receiver.
- Anisole is the second most volatile among the four and it will start to vaporize after propionic acid as the temperature will increase with time and it will be collected in the second distillate liquid receiver.
- Propionic Anhydride in the third receiver.
- 4-Methoxypropiophenone will be left in the reactor and can be taken out.


batchdisttilation.apwz - Aspen Plus V14 - aspenONE
Time
hr
fraction
ANISOLE
PROPI-01
PROPI-02
MPP
NITROGEN
6.4 0.488679 0.130149 0.381172 0
6.5 0.496488 0.135307 0.368206 0
6.6 0.50395 0.140479 0.35557 0
6.7 0.511063 0.145673 0.343264 0
6.8 0.517823 0.150892 0.331285 0
6.9 0.524226 0.156143 0.319631 0
7 0.530269 0.161433 0.308299 0
7.1 0.535947 0.166768 0.297285 0
7.2 0.541256 0.172158 0.286586 0
7.3 0.546189 0.177613 0.276198 0
7.4 0.550742 0.18314 0.266118 0
7.5 0.554907 0.188752 0.256341 0
7.6 0.558679 0.194459 0.246862 0
7.7 0.562048 0.200275 0.237678 0
7.8 0.565006 0.206211 0.228783 0
7.9 0.567544 0.212282 0.220173 0
8 0.569653 0.218502 0.211844 0
8.1 0.571323 0.224886 0.203792 0
8.2 0.572541 0.231447 0.196012 0
FEED
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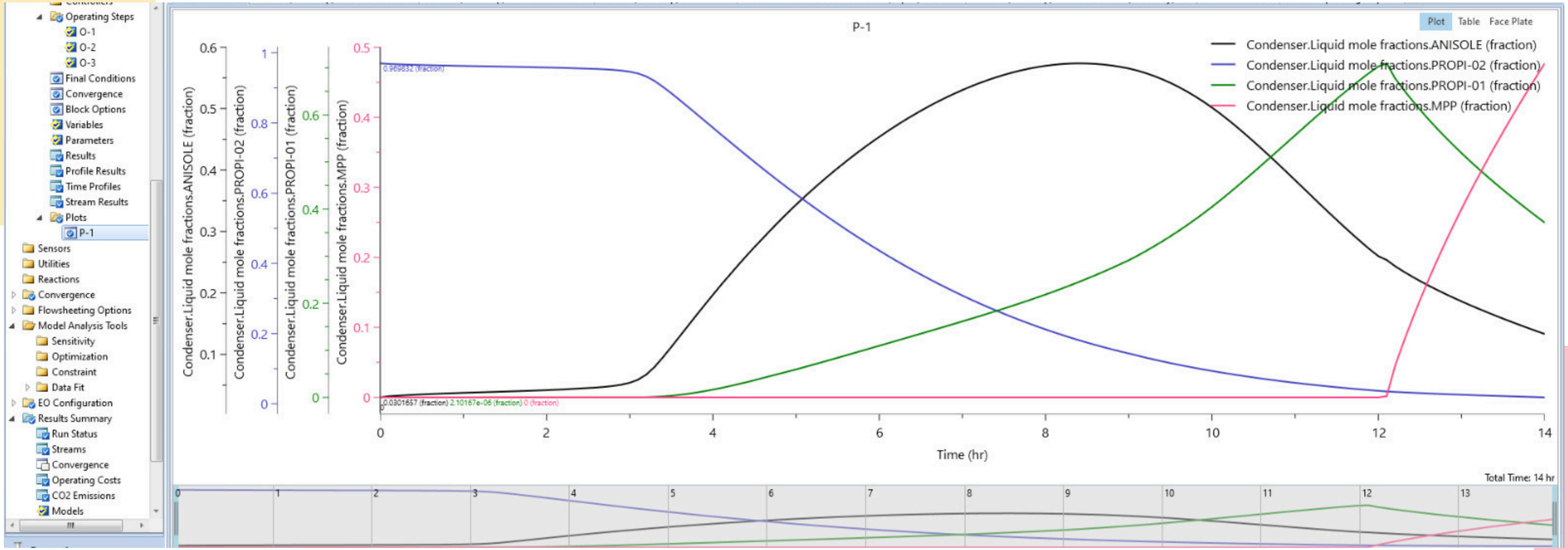
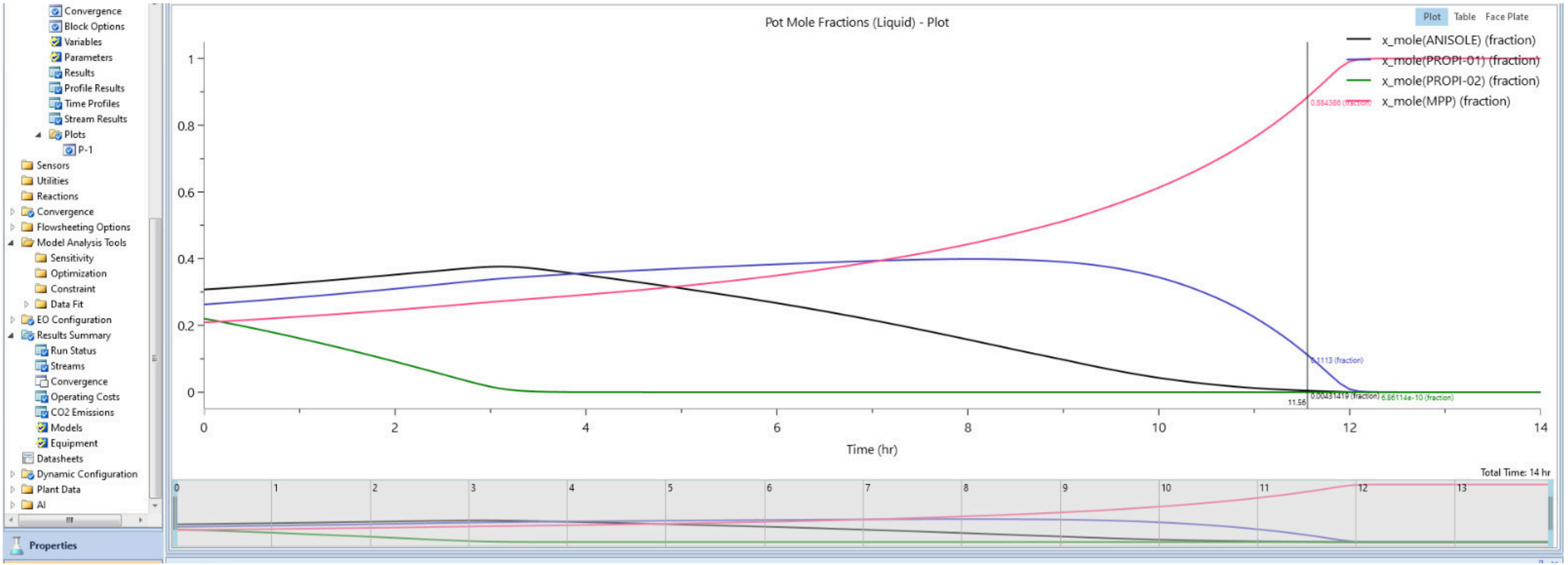


Condenser liquid mole fraction vs Time.

- The concentration of propionic acid firstly increases then decreases.
- Then the concentration of anisole increases and then decreases.
- Then the concentration of propionic anhydride increases in the condenser. By this method, we can separate the compounds.



Reactor mole fraction vs time

As the three volatile compounds vapourizes, their concentration decreases with the time in the reactor 4-Methoxypropiophenone is left almost alone in the reactor which can be further used in the production of Anethole.

Recommendations:

- Increasing pressure of the condenser helps in better separation by increasing the difference in boiling point of components of nearly the same volatility.
- Increase in stages helps in better separation of compounds.
- Increase in reflux ratio increases the amount of liquid on the trays which helps to improve the separation of the components. But, increasing reflux ratio reduces the amount of product that is withdrawn from the column

THANK YOU