SIMUTECH PROJECT REPORT

HANDS-ON
ASPEN AND MATLAB

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210009

OVERVIEW

- Differential equations are essential for modeling and analyzing dynamic systems.

- MATLAB provides powerful tools for numerically solving differential equations.

- This report explores the utilization of MATLAB in solving differential equations and its application in heat conduction problems in chemical engineering.

- The report also discusses the use of Aspen, a process simulation software, for solving reactor problems.

- The report is organized as follows:

  - Introduction to differential equations and MATLAB's capabilities in solving ordinary and partial differential equations.

  - Application of MATLAB in solving heat conduction problems in chemical engineering, including formulation, boundary conditions, and real-world case studies.

  - Introduction to Aspen and its role in modeling and simulating various reactor problems.

  - Practical application of Aspen for solving reactor problems, including a step-by-step guide and analysis of simulation outcomes.

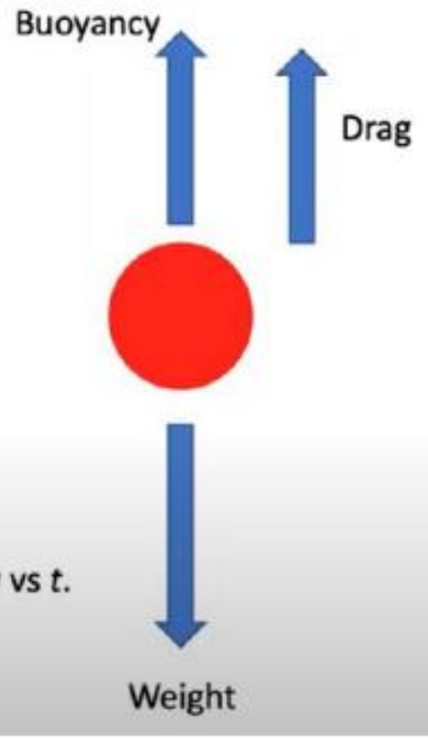
  - Presentation of case studies demonstrating the combined usage of MATLAB and Aspen.

ASSIGNMENT 1 : PROBLEM STATEMENT

Assignment 1

$$m\frac{du}{dt} = W - F_B - F_D$$

$$m\frac{du}{dt} = mg - V\rho g - 6\pi R\eta u$$



EXERCISE:

- ❑ Fix the properties of the fluid and solid sphere.
- ❑ Do you get a terminal velocity? What will be the analytical expression for the same?
- ❑ Get the analytical answer for u vs t (assume $u = 0$ at $t = 0$)
- ❑ For the same initial velocity, numerically compute u vs t.
- ❑ Compare the analytical and numerical answers on a plot of u vs t.
    - ❑ Analytical – solid line; numerical – dashed line

➢ Take the value of the required properties as follows:

- Radius of sphere = 10^{-5} m
- Density of liquid = 1000 kg/m^3
- Density of sphere = 8050 kg/m^3
- Viscosity of liquid = 10^{-3} Pa.s
- Acceleration due to gravity = 9.8 m/s

→ To calculate analytical expression for u vs t

⇒ The equation of motion for an object falling through a viscous fluid is given by

$$m\frac{du}{dt} = mg - 6\pi\eta R u$$

where u is velocity of sphere at time t

Taking $m = \sigma V$ where σ = density of sphere
V = volume of sphere

$$\Rightarrow \sigma V\frac{du}{dt} = w/\,Vg - 6\pi\eta R u$$

$$\Rightarrow \sigma V\frac{du}{dt} = \sigma Vg - \rho Vg - 6\pi\eta R v$$

$$\Rightarrow \sigma V\frac{du}{dt} = (\sigma - \rho)Vg - 6\pi\eta R u$$

$$\Rightarrow \int_0^t \frac{dt}{\sigma V} = \int_0^u \frac{du}{(\sigma-\rho)Vg - 6\pi\eta R V}$$

$$\Rightarrow \frac{t}{\sigma V} = \frac{\ln[(\sigma-\rho)Vg - 6\pi\eta R u)]_0^u}{-6\pi\eta R}$$

SOLUTION:

Numerical computation of u vs t:

To obtain the numerical solution for u vs t, we can use numerical integration techniques such as Euler's method or the Runge-Kutta method. By discretizing the time interval and approximating the derivative, we can calculate the velocity at each time step.

Comparison of analytical and numerical answers:

Plotting the analytical solution (solid line) and the numerical solution (dashed line) on the same graph will allow us to compare the two solutions and observe any differences or similarities between them.

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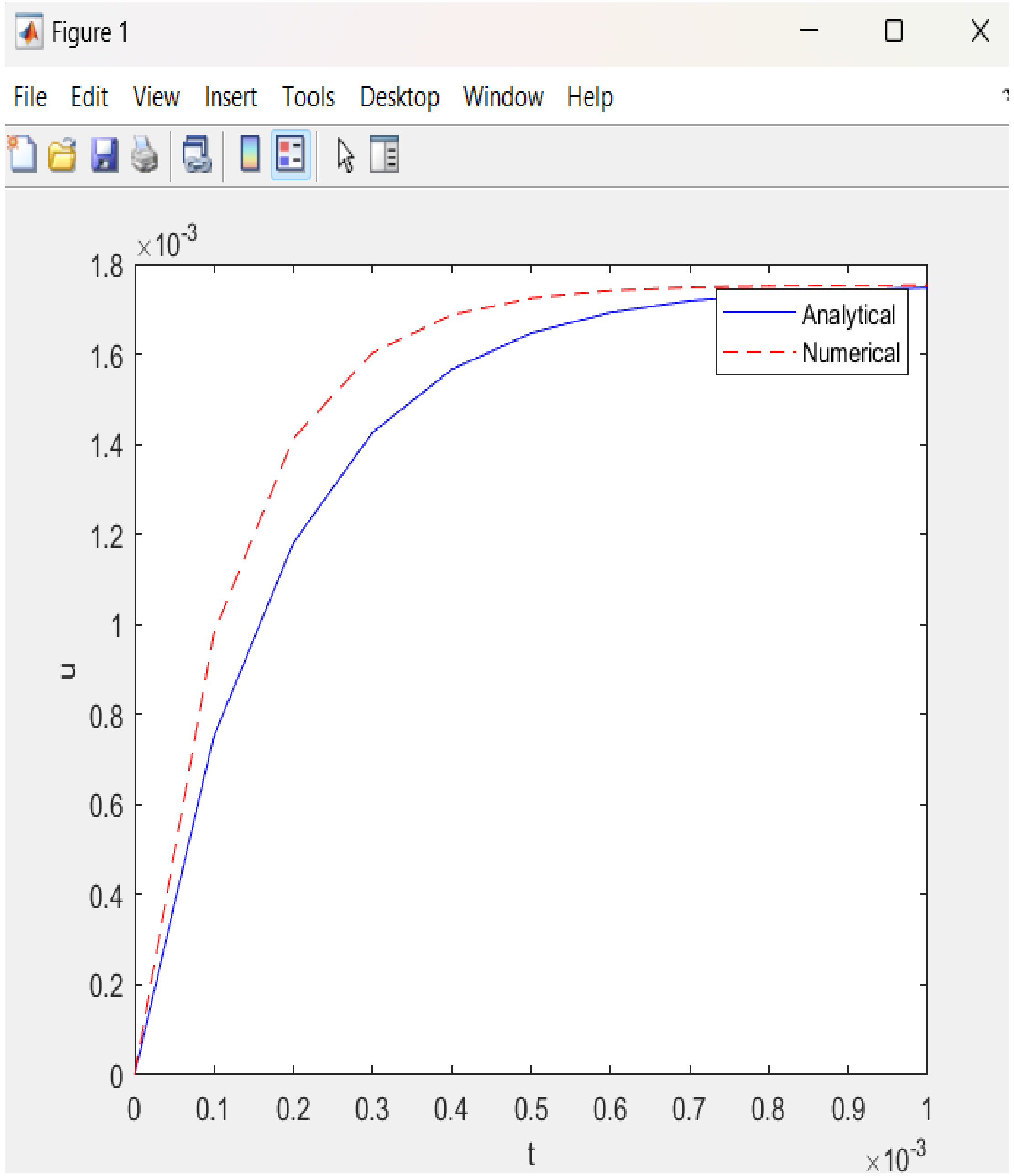
amc... | untit... | MAT... | ass1... | ass1...

```matlab
% Define the parameters
density = 8050;    % Density of the sphere material
r = 0.00001;       % Radius of the sphere
m = (4/3) * pi * r^3 * density; % Mass of the sphere
g = 9.8;           % Acceleration due to gravity
mu = 0.001;        % Viscosity of the fluid

% Define the time interval
dt = 0.0001;
t = 0:dt:0.001;

% Initialize arrays for storing velocity values
u_analytical = zeros(size(t));
u_numerical = zeros(size(t));

% Analytical solution
u_analytical = (m * g) / (6 * pi * r * mu) * (1 - exp(-(6 * pi * r * mu * t) / m));

% Numerical solution using Euler's method
u_numerical(1) = 0;
for i = 2:length(t)
    u_numerical(i) = u_numerical(i - 1) + (((m * g) - (6 * pi * r * mu * u_numerical(i - 1))) / m) * dt;
end

% Plotting the results
plot(t, u_analytical, 'b-', t, u_numerical, 'r--');
xlabel('t');
ylabel('u');
legend('Analytical', 'Numerical');
```



ASSIGNMENT 2: PROBLEM STATEMENT

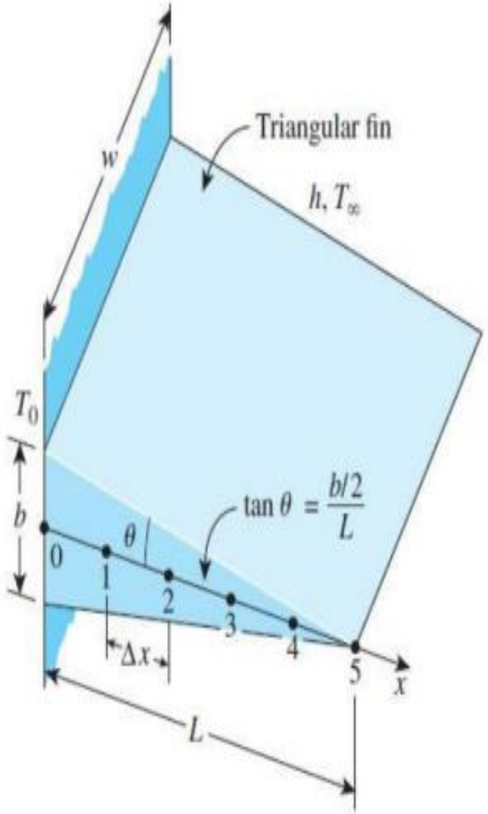
Assignment-2

Consider an aluminum alloy fin (k = 180 W/m·K) of triangular cross section with length L=20 cm, base thickness b = 4 cm, and very large width w. The base of the fin is maintained at a temperature of T_0 = 100°C. The fin is losing heat to the surrounding medium at T_∞ =25°C with a heat transfer coefficient of h = 15 W/m2·K. Using the finite difference method with 20 equally spaced nodes along the fin in the x-direction,

Write a matlab program to find-

(a) The Temperatures at the nodes

(b) Plot the Temperature(T) vs distance from the base(x) plot.



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amc... ×
untit... ×
MAT... ×
ass1... ×
ass1... ×
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+

```
A=zeros(20,20);
B=zeros(20,1);

for i=2:20
    B(i,1)=-0.209;
end
B(1,1) = -1950.209;

for i=2:1:19
   A(i,i-1)=20.5-i;
   A(i,i)=2*(i) - 40.008;
   A(i,i+1)=19.5-(i);

end
A(1,1)=2*(1) - 40.008;
A(1,2)=19.5-(1);
A(20,19)=1;
A(20,20)=-1.008;

A
B
maxerr = 1e-5;
T = zeros(1,size(A,1));
err1 = inf;
itr = 0;
while all(err1>maxerr)
    T_old = T;
    for i = 1:size(A,1)
        sum = 0;
        for j = 1:i-1
            sum = sum + A(i,j)*T(j);
        end
        for j=i+1:size(A,1)
        sum = sum+A(i,j)*T_old(j);
        end
        T(i) = (1/A(i,i)) * (B(i) - sum);
    end
    itr = itr + 1;
    y(itr,:) = T;
    err1 = abs(T_old-T);
end
for i=1:1:20
    fprintf("T_%d is %d.\n",i,T(i));
end
x=0.01:0.01:0.2;
plot(x,T)
```

```
T_1 is 9.945220e+01.
T_2 is 9.890652e+01.
T_3 is 9.836296e+01.
T_4 is 9.782152e+01.
T_5 is 9.728221e+01.
T_6 is 9.674502e+01.
T_7 is 9.620997e+01.
T_8 is 9.567703e+01.
T_9 is 9.514624e+01.
T_10 is 9.461757e+01.
T_11 is 9.409103e+01.
T_12 is 9.356663e+01.
T_13 is 9.304435e+01.
T_14 is 9.252421e+01.
T_15 is 9.200621e+01.
T_16 is 9.149034e+01.
T_17 is 9.097661e+01.
T_18 is 9.046504e+01.
T_19 is 8.995571e+01.
T_20 is 8.944911e+01.
```

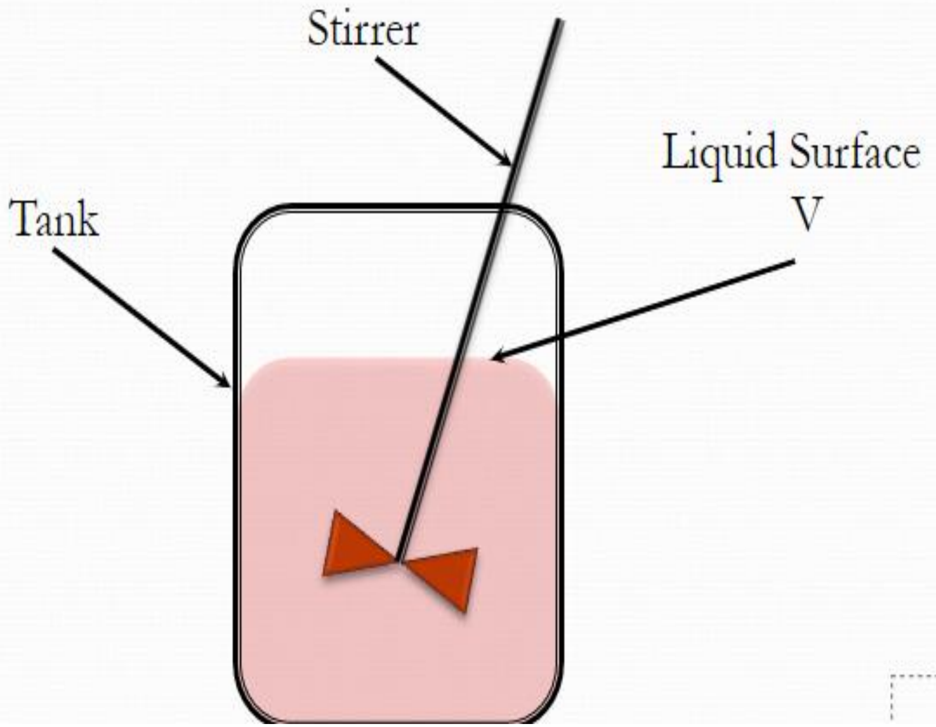
Reactors:

Batch Reactor:

Definition:

Batch Reactors are defined as reactors in which no flow of mass across the reactor boundaries, once the reactants have been charged.

Schematic Representation of Batch Reactors:



Continuous Stirred Tank Reactor (CSTR):

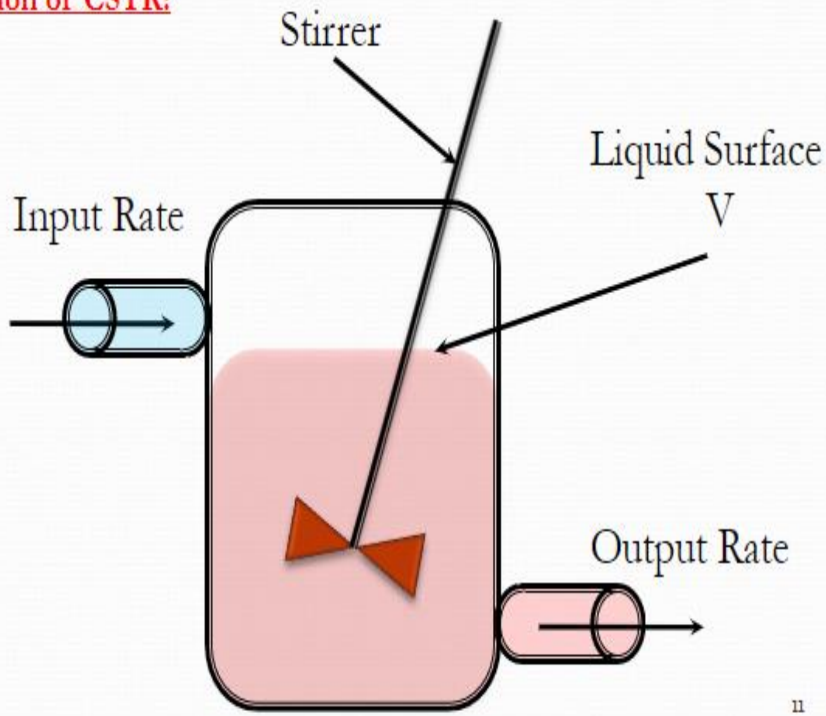
Definition:

Continuous Stirred Tank Reactors (CSTR) are defined to be flow reactors characterized by intense mixing so that the properties anywhere inside the reactor are exactly the same as that of the exist stream.

Schematic Representation of CSTR:

This model can be used to:

1. model a bed of catalyst powder, i.e. fluidized-bed reactors.
2. Slurry bubble column reactor
3. Polymerization reactors



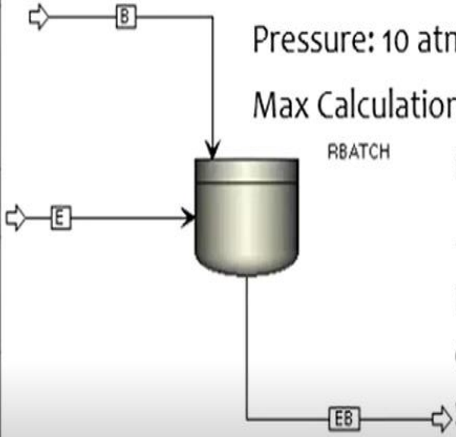
BATCH REACTOR:

Problem Description:

The specific chemistry used to illustrate the use of Aspen Plus is the reaction of ethylene (E) with benzene (B) to form ethylbenzene (EB)

$$C_2H_4 \text{ (Ethylene)} + C_6H_6 \text{ (Benzene)} \rightarrow C_8H_{10} \text{ (Ethylbenzene)}$$

Feed Condition (SI units)	Ethylene	Benzene
Temp. (K)	298	300
Pressure (atm)	15	15
Molar Flow(kmole/hr)	50	100



Reactor Spec.

Batch feed time: 1 hour

Pressure: 10 atm

Max Calculation time: 2 hrs

Rate of reaction

$$-r_A = C_E C_B (1.528\text{x } 10^8) e^{\frac{(-7.1129\text{x}10^7)}{RT}}$$

Fluid Package

CHAO-SEA

Specific Reaction Rate Constant

$K = K_o \exp(-E_a/RT)$

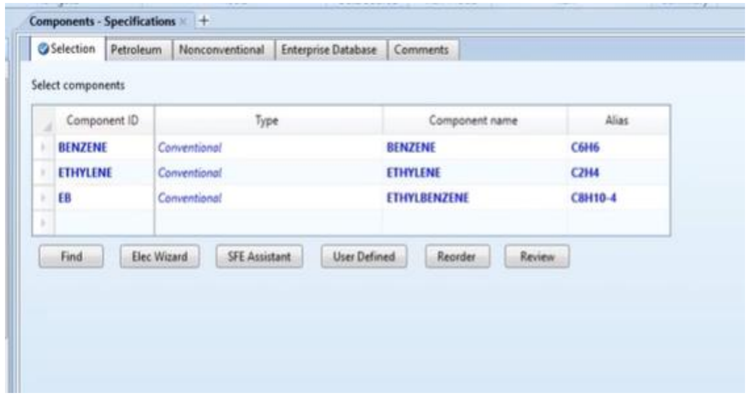
Ko= 1.528e6 kmol/s.m3

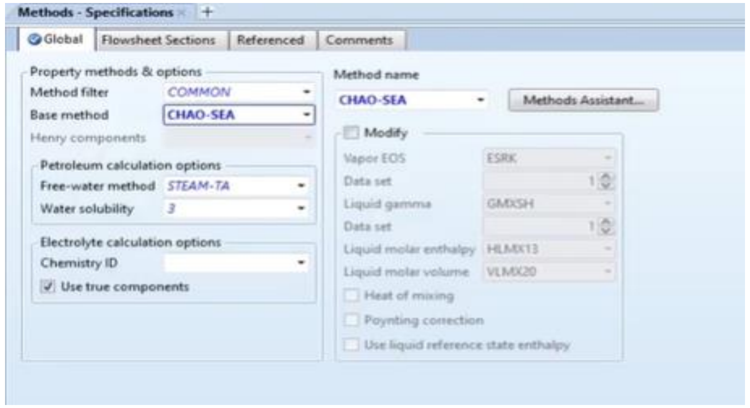
Ea= $7.1129\text{x}10^7$ J/kmol

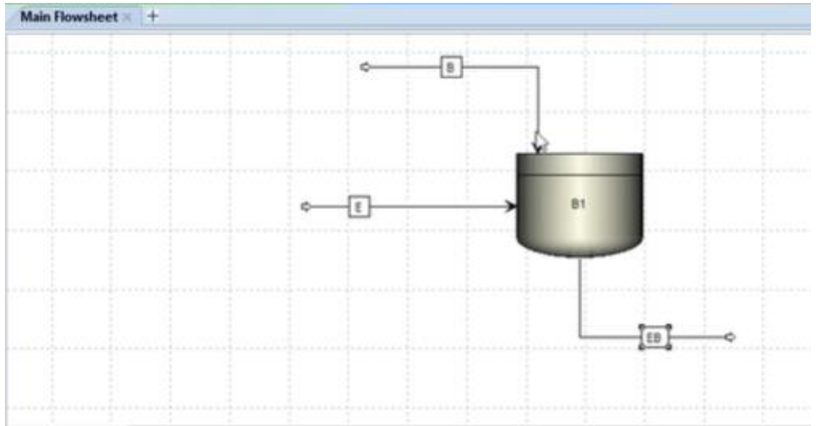
OBJECTIVES:

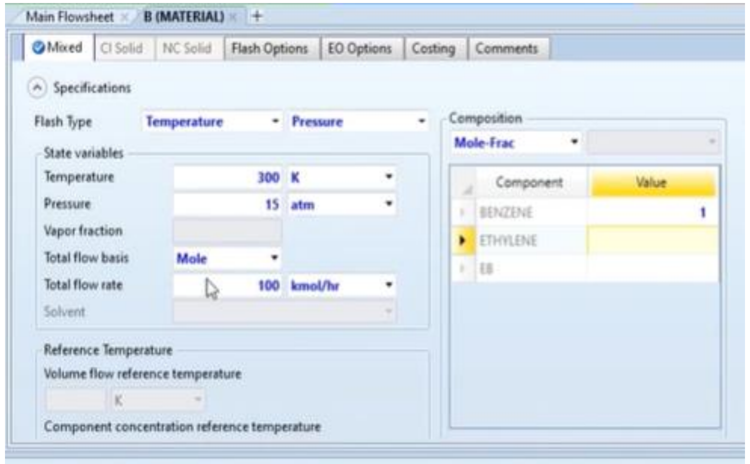
- **ANALYZE:** The concentration of reactants and products as a function of time.
- **PLOT:** The temperature profile

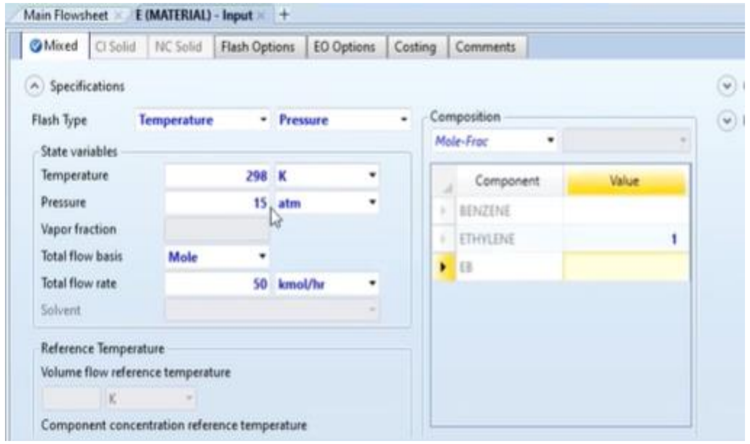
SOLUTION STEPS:

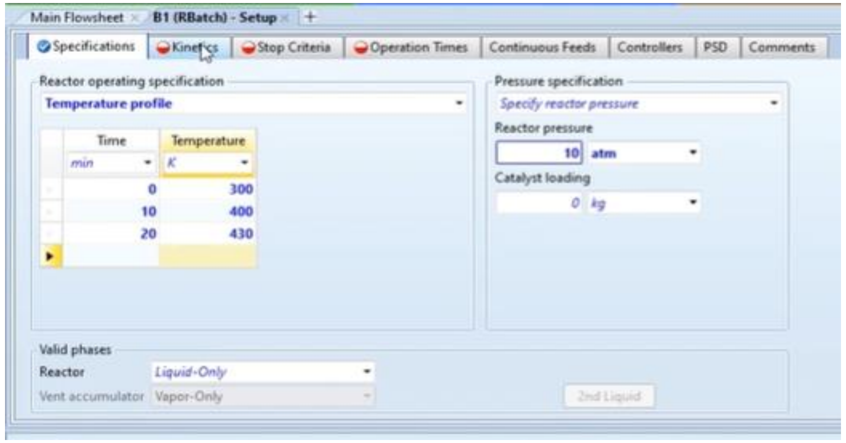


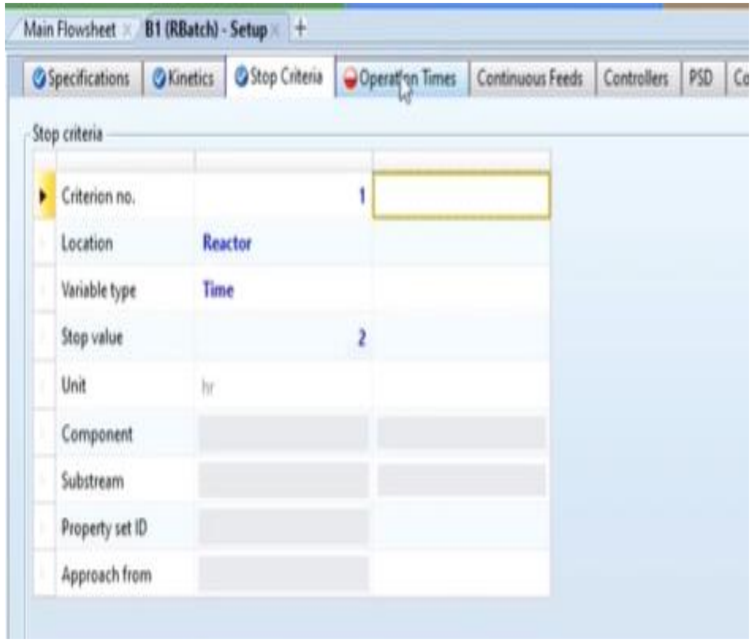


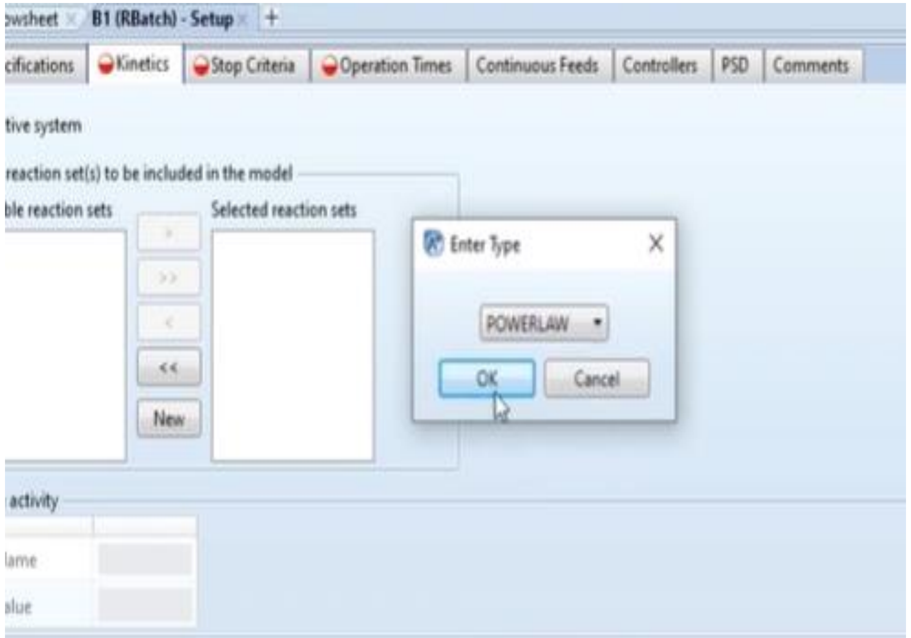


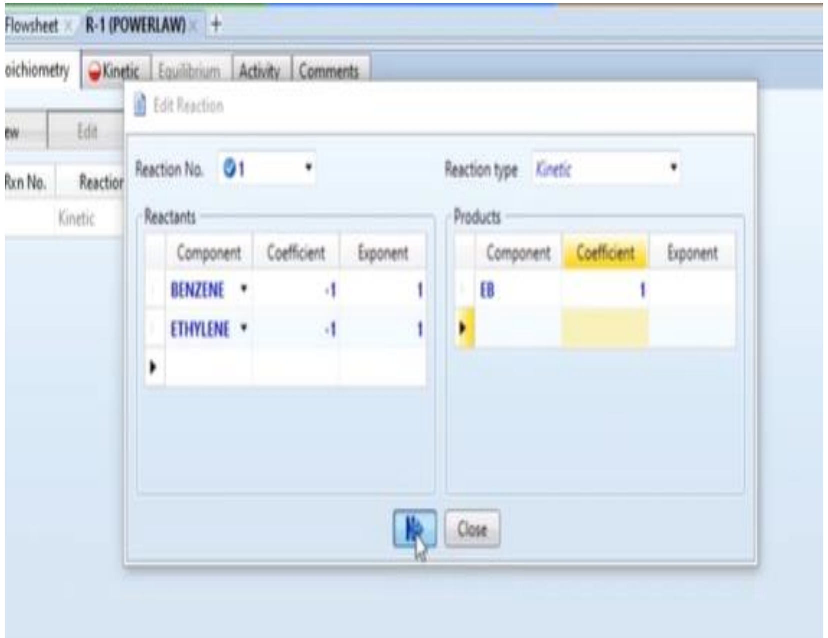


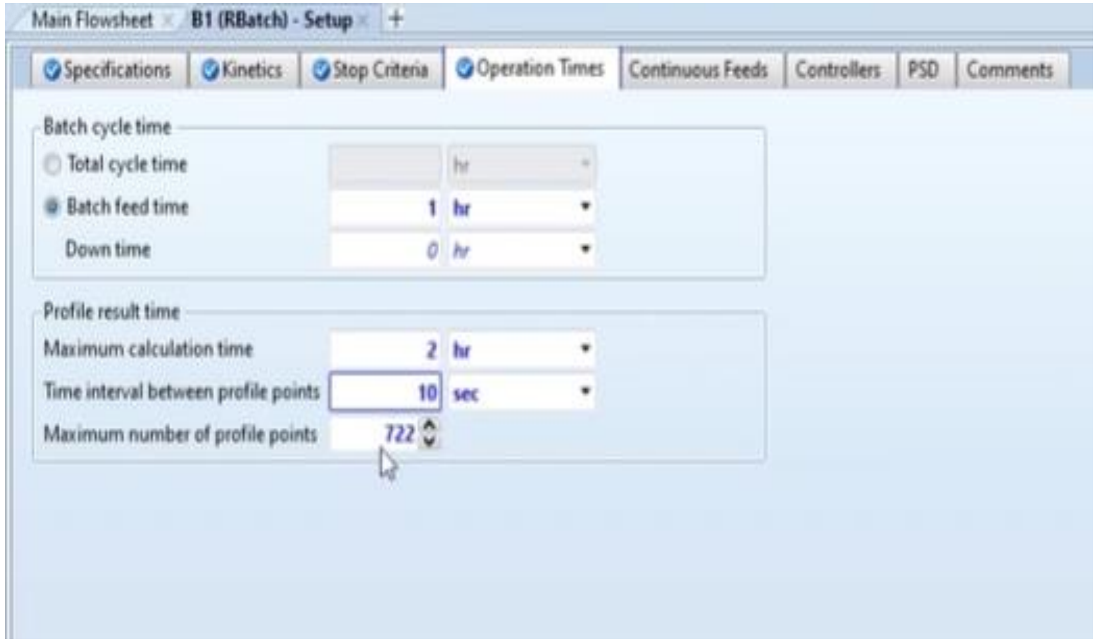


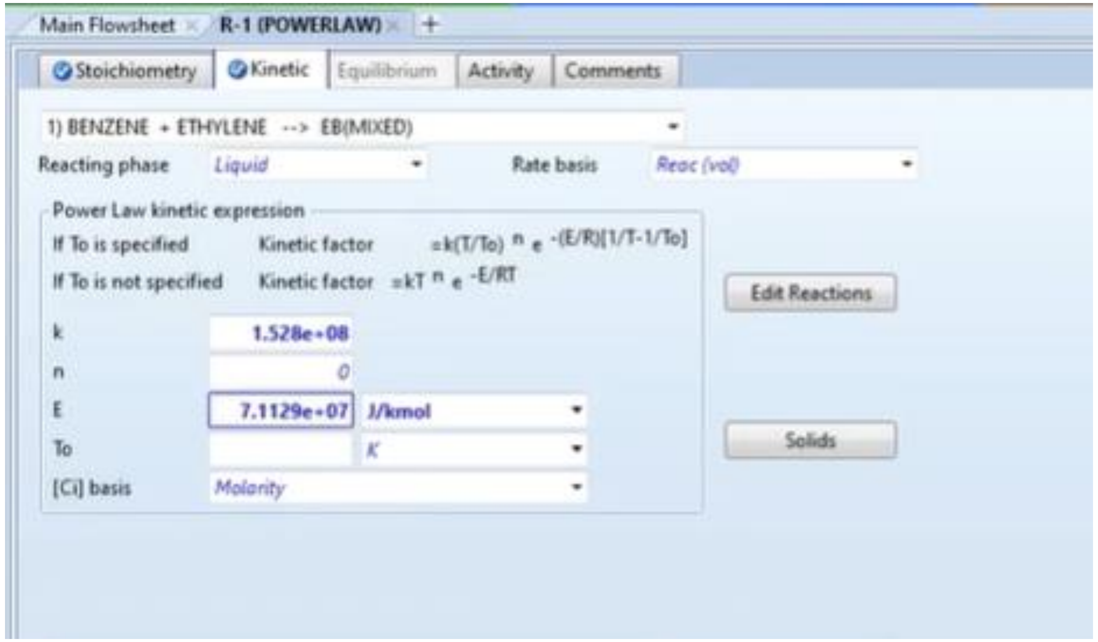



Main Flowsheet
B1 (RBatch) - Setup
Specifications
Kinetics
Stop Criteria
Operation Times
Continuous Feeds
Controllers
PSD
Stop criteria
Criterion no. 1
Location Reactor
Variable type Time
Stop value 2
Unit hr
Component
Substream
Property set ID
Approach from

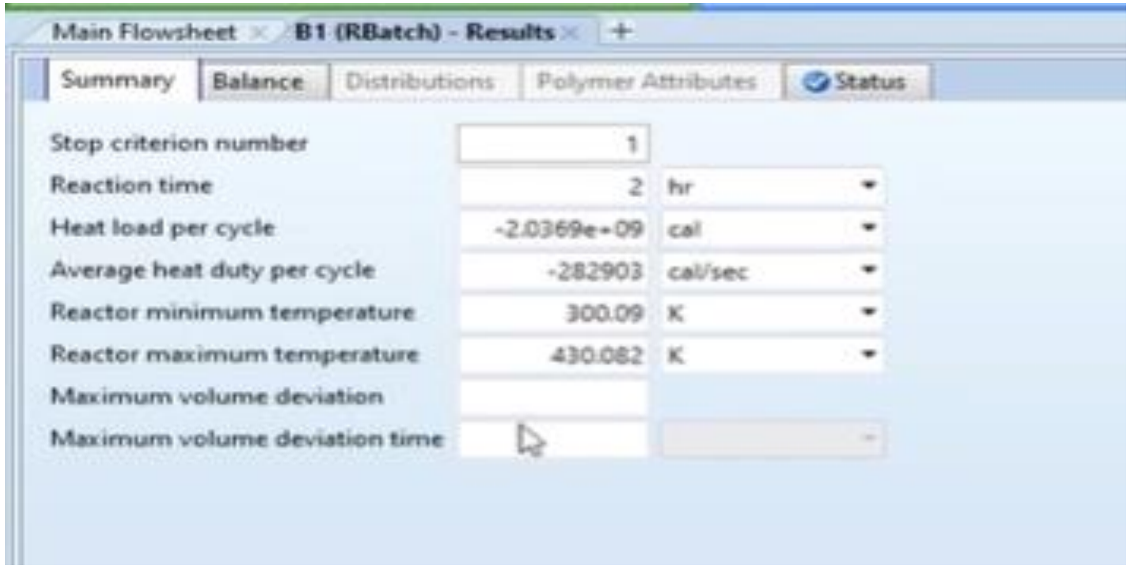

B1 (RBatch) - Setup
Kinetics
Stop Criteria
Operation Times
Continuous Feeds
Controllers
PSD
Comments
reaction set(s) to be included in the model
Selected reaction sets
New
Enter Type
POWERLAW
OK
Cancel
activity

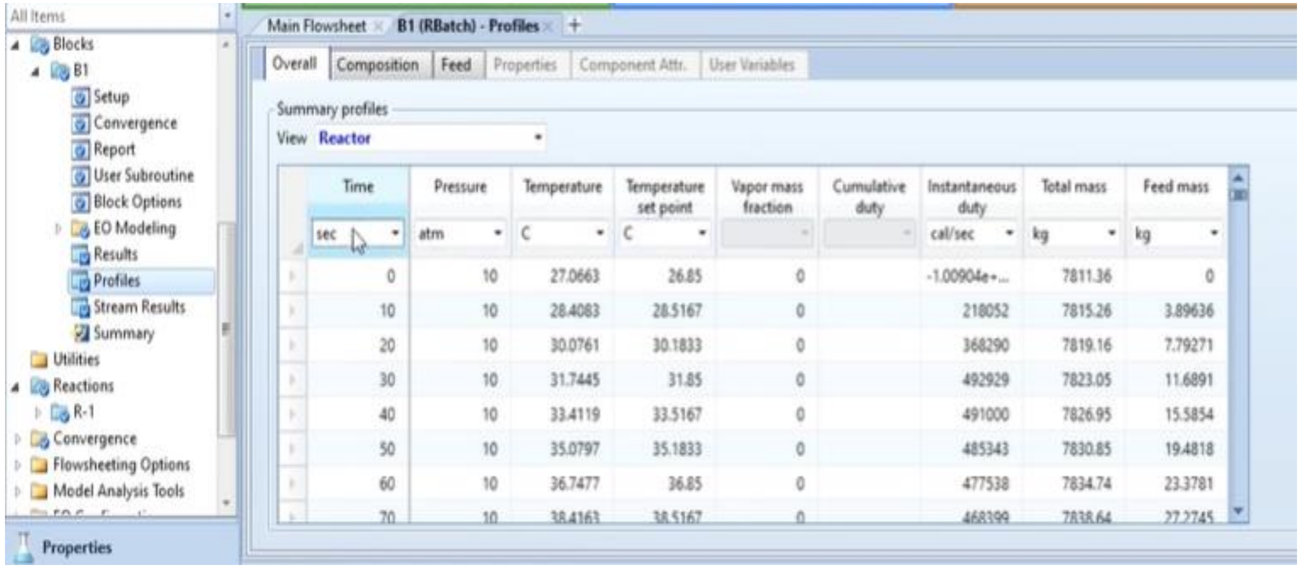

R-1 (POWERLAW)
Kinetic
Equilibrium
Activity
Comments
Edit Reaction
Reaction No. 1
Reaction type Kinetic
Reactants
Component
Coefficient
Exponent
BENZENE -1 1
ETHYLENE -1 1
Products
EB 1
Close


Main Flowsheet
B1 (RBatch) - Setup
Specifications
Kinetics
Stop Criteria
Operation Times
Continuous Feeds
Controllers
PSD
Comments
Batch cycle time
Total cycle time hr
Batch feed time 1 hr
Down time 0 hr
Profile result time
Maximum calculation time 2 hr
Time interval between profile points 10 sec
Maximum number of profile points 722

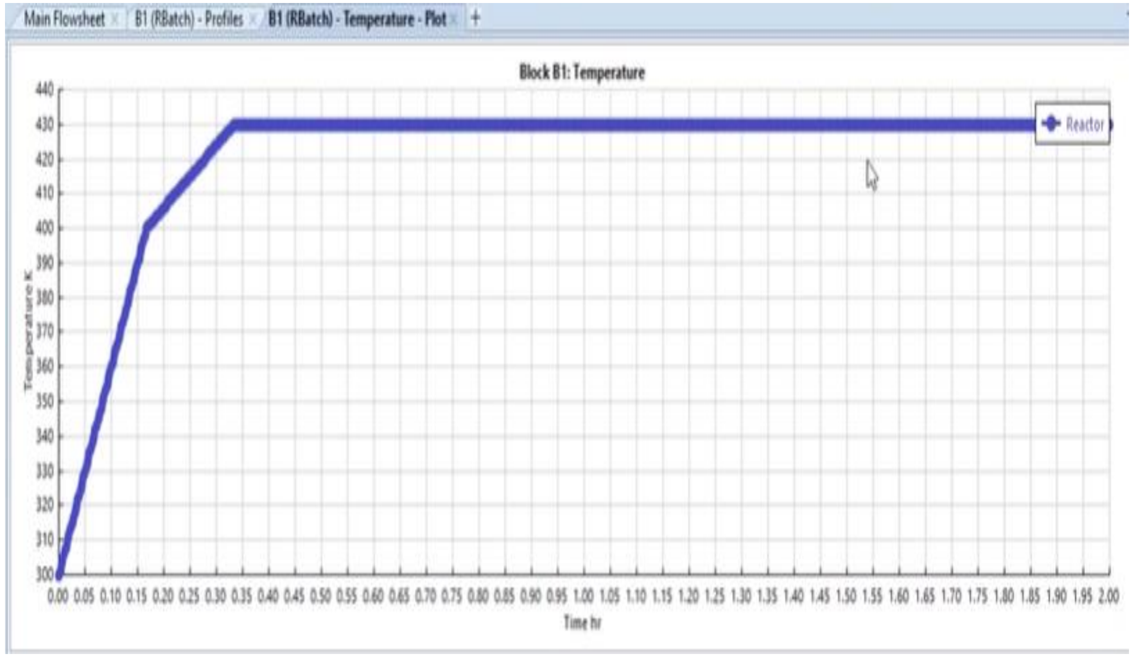

Main Flowsheet
R-1 (POWERLAW)
Stoichiometry
Kinetic
Equilibrium
Activity
Comments
1) BENZENE + ETHYLENE --> EB(MIXED)
Reacting phase Liquid
Rate basis Reac (vol)
Power Law kinetic expression
If To is specified Kinetic factor =k(T/To) n e -(E/R)[1/T-1/To]
If To is not specified Kinetic factor =kT n e -E/RT
Edit Reactions
k 1.528e+08
n 0
E 7.1129e+07 J/kmol
To K
[Ci] basis Molarity
Solids

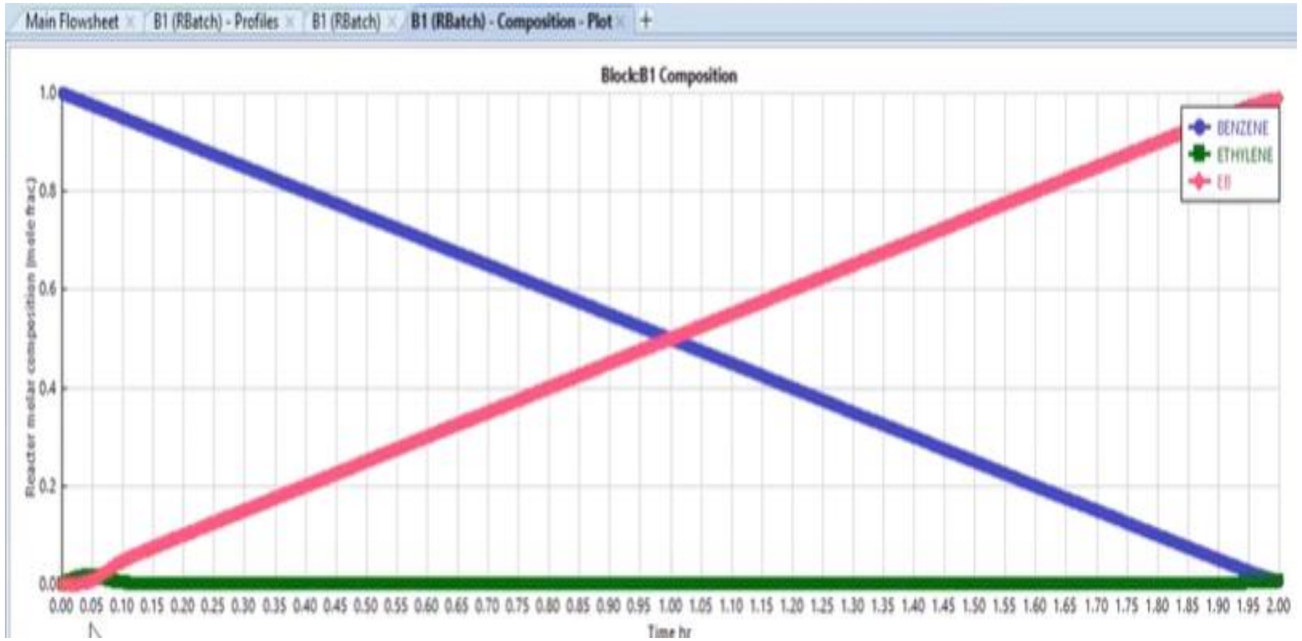
RESULTS AND ANALYSIS:





Time	Pressure	Temperature	Temperature set point	Vapor mass fraction	Cumulative duty	Instantaneous duty	Total mass	Feed mass
sec	atm	C	C			cal/sec	kg	kg
0	10	27.0663	26.85	0		-1.00904e+...	7811.36	0
10	10	28.4083	28.5167	0		218052	7815.26	3.89636
20	10	30.0761	30.1833	0		368290	7819.16	7.79271
30	10	31.7445	31.85	0		492929	7823.05	11.6891
40	10	33.4119	33.5167	0		491000	7826.95	15.5854
50	10	35.0797	35.1833	0		485343	7830.85	19.4818
60	10	36.7477	36.85	0		477538	7834.74	23.3781
70	10	38.4163	38.5167	0		468399	7838.64	27.2745





CSTR REACTOR:

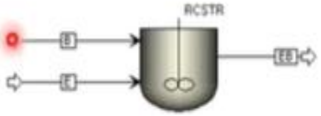
Case. RCSTR Reactor Design

Problem Description:

- The specific chemistry used to illustrate the use of Aspen Plus is the reaction of ethylene (E) with benzene (B) to form ethylbenzene (EB)

C_2H_4 (Ethylene) + C_6H_6 (Benzene) → C_8H_{10} (Ethylbenzene)

Feed Condition (SI units)	Ethylene	Benzene
Temp. (K)	298	300
Pressure (atm)	15	15
Molar Flow(kmole/hr)	50	100



Reactor Spec.

Reactor Temp 400K

Pressure: 10 atm

Reactor Volume 0.1 cum

Rate of reaction

$-r_A = C_E C_B (1.528x\,10^8) e^{\frac{(-7.1129x10^7)}{RT}}$

Fluid Package

CHAO-SEA

Specific Reaction Rate Constant

$K = K_o \exp(-E_a/RT)$

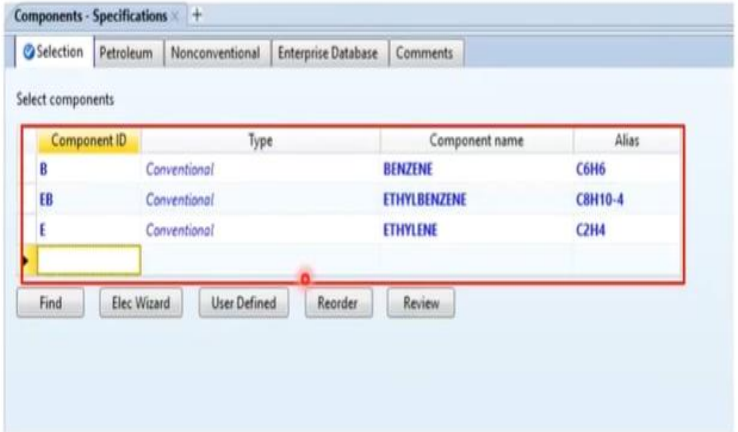
Ko= 1.528e8 kmol/s.m3

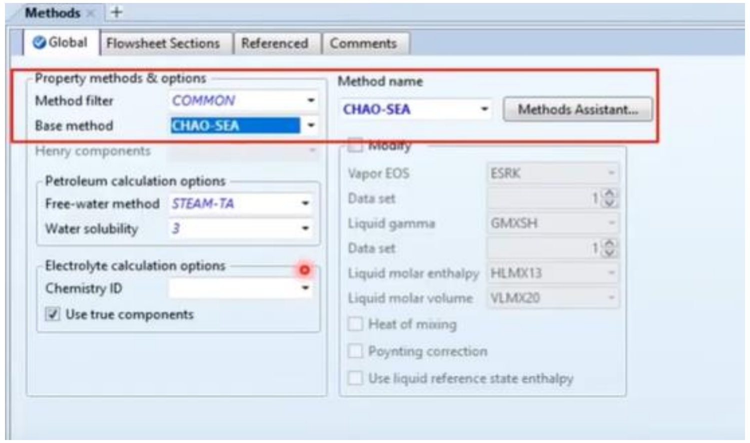
Ea= $7.1129x10^7$ J/kmol

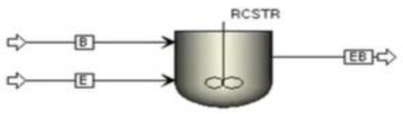
OBJECTIVES:

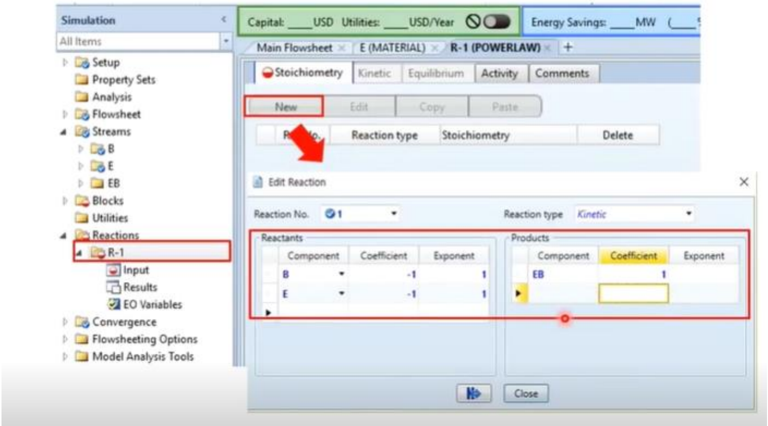
- **ANALYZE:** as Using Design specs to analyze the volume of the reactor for 98% ethylene conversion.
- **CALCULATE:** The conversion of ethylene for given reaction kinetics.

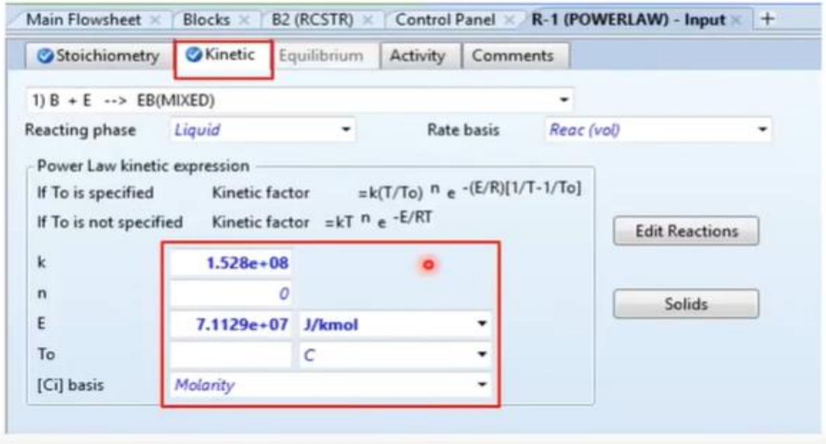
SOLUTION STEPS:

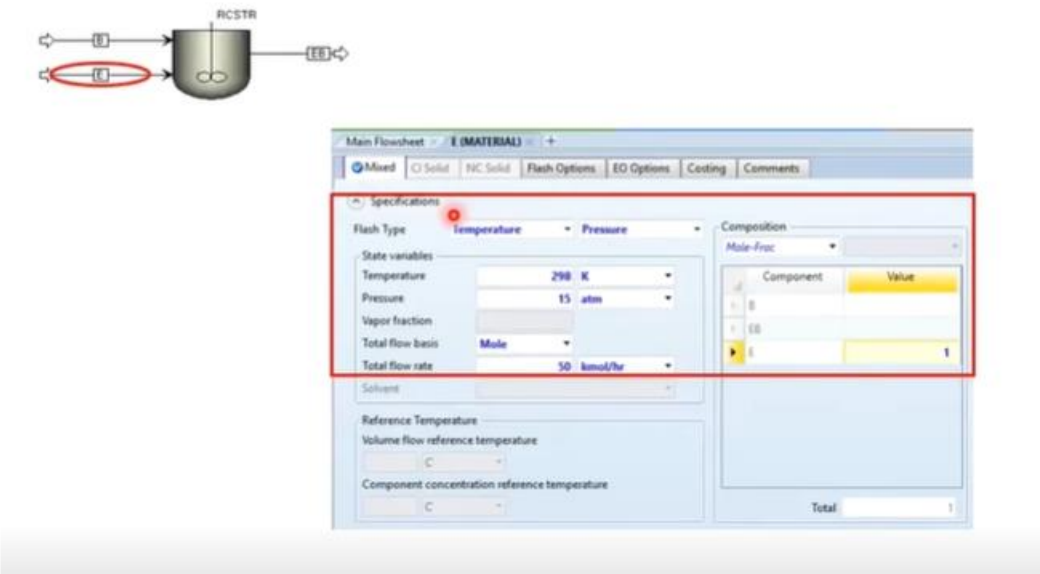


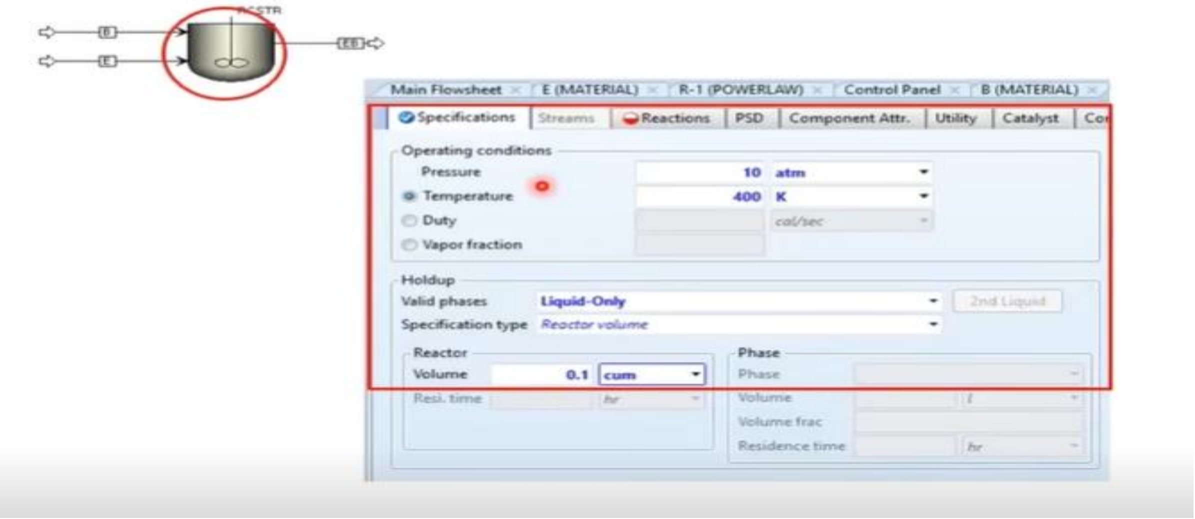


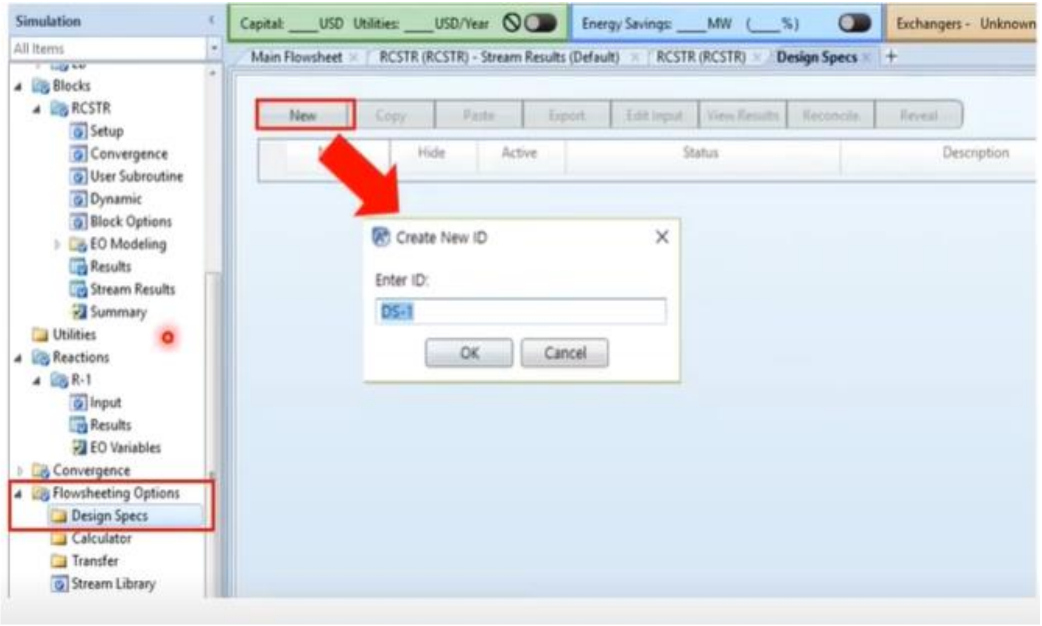


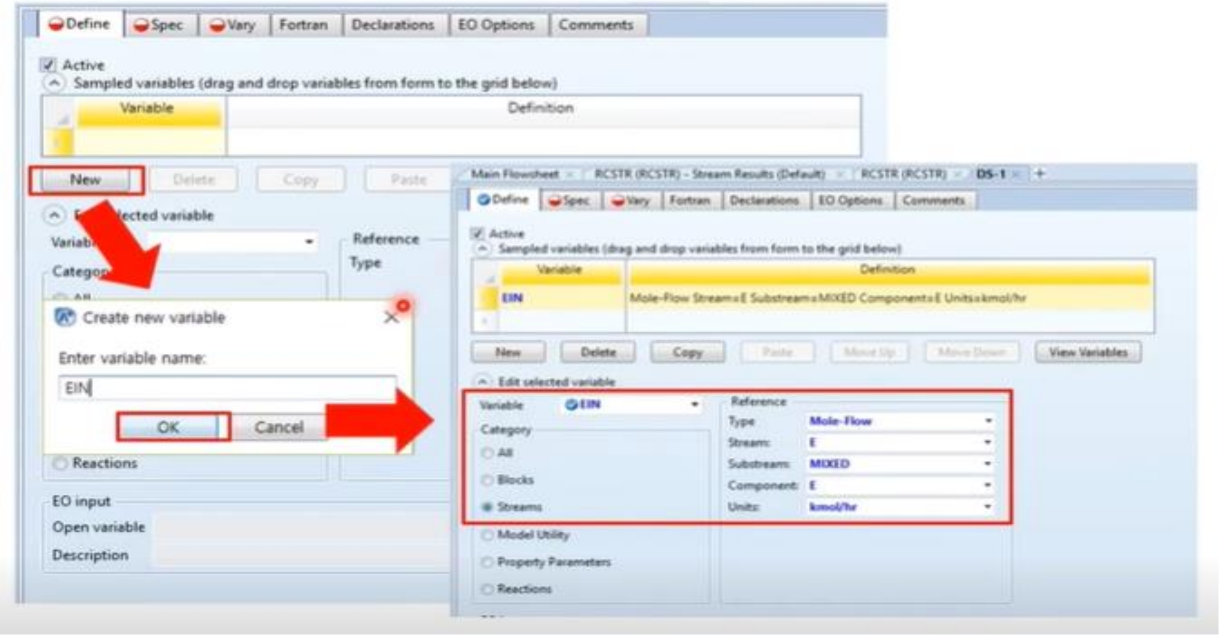


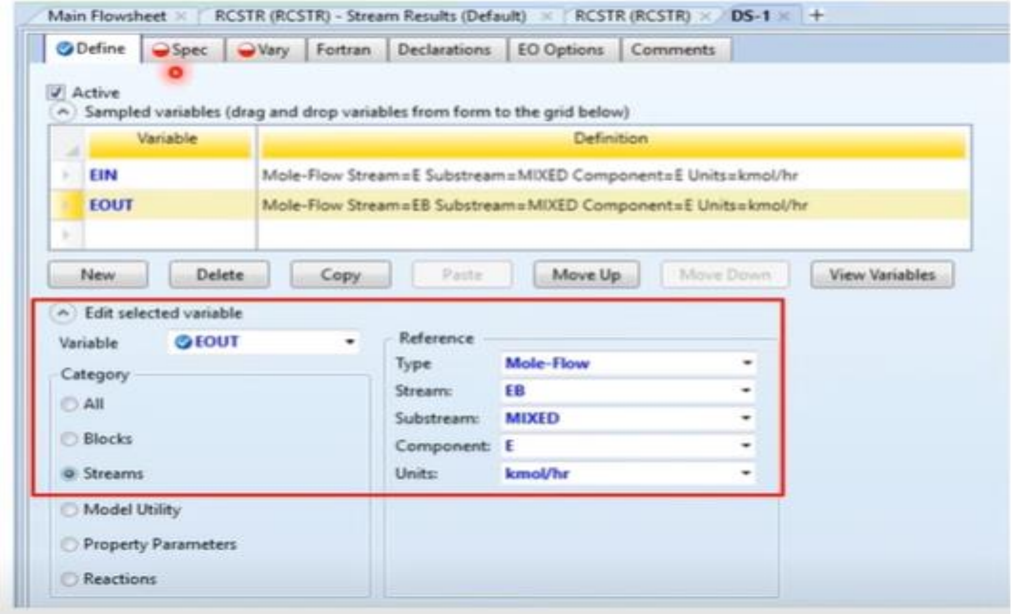


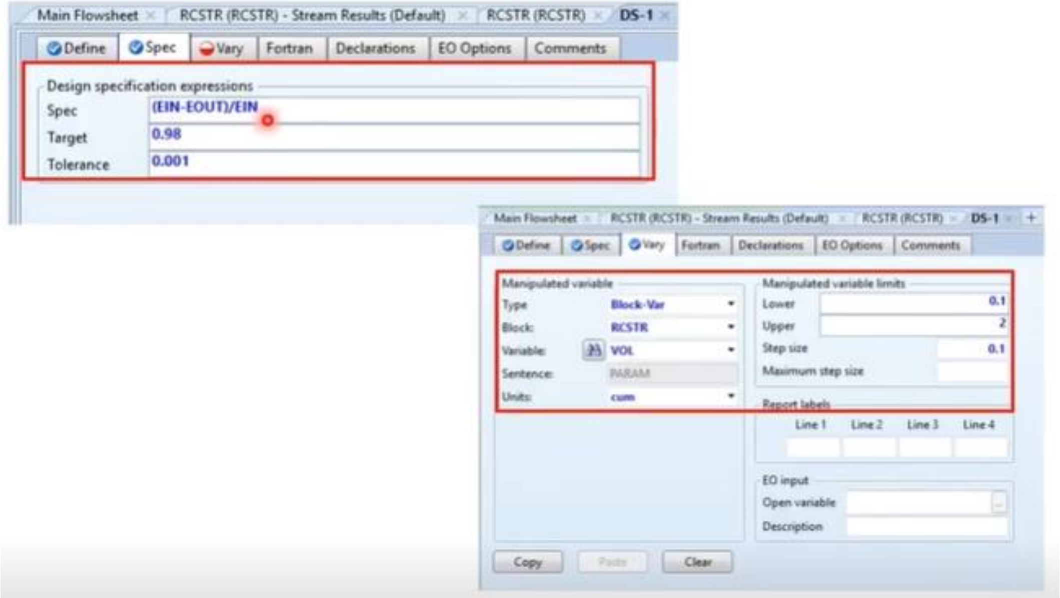

RCSTR
Main Flowsheet
E (MATERIAL)
Mixed
CI Solid
NC Solid
Flash Options
EO Options
Costing
Comments
Specifications
Flash Type
Temperature
Pressure
Composition
Mole-Frac
State variables
Temperature
298
K
Pressure
15
atm
Vapor fraction
Total flow basis
Mole
Total flow rate
50
kmol/hr
Solvent
Component
Value
1
Reference Temperature
Volume flow reference temperature
C
Component concentration reference temperature
C
Total
1


RCSTR
Main Flowsheet
E (MATERIAL)
R-1 (POWERLAW)
Control Panel
B (MATERIAL)
Specifications
Streams
Reactions
PSD
Component Attr.
Utility
Catalyst
Operating conditions
Pressure
10
atm
Temperature
400
K
Duty
cal/sec
Vapor fraction
Holdup
Valid phases
Liquid-Only
2nd Liquid
Specification type
Reactor volume
Reactor
Volume
0.1
cum
Resi. time
hr
Phase
Phase
Volume
Volume frac
Residence time
hr

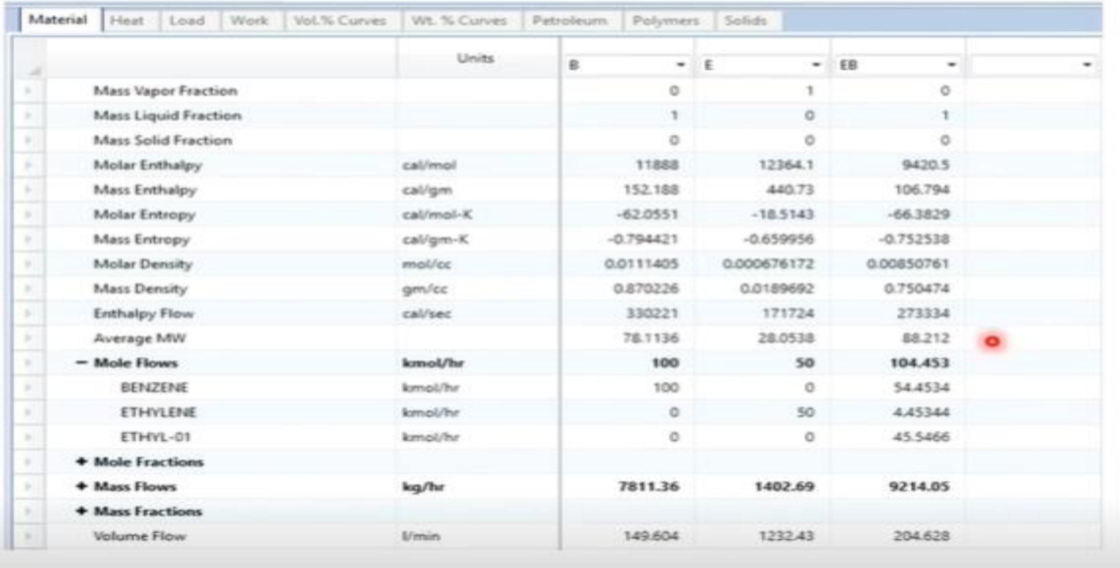

Simulation
All Items
Blocks
RCSTR
Setup
Convergence
User Subroutine
Dynamic
Block Options
EO Modeling
Results
Stream Results
Summary
Utilities
Reactions
R-1
Input
Results
EO Variables
Convergence
Flowsheeting Options
Design Specs
Calculator
Transfer
Stream Library
Capital: ___USD Utilities: ___USD/Year
Energy Savings: ___MW (___%)
Exchangers - Unknown
Main Flowsheet
RCSTR (RCSTR) - Stream Results (Default)
RCSTR (RCSTR)
Design Specs
New
Copy
Paste
Export
Edit Input
View Results
Reconcile
Reveal
Hide
Active
Status
Description
Create New ID
Enter ID:
DS-1
OK
Cancel


Define
Spec
Vary
Fortran
Declarations
EO Options
Comments
Active
Sampled variables (drag and drop variables from form to the grid below)
Variable
Definition
New
Delete
Copy
Paste
Reference
Type
Create new variable
Enter variable name:
EIN
OK
Cancel
Reactions
EO input
Open variable
Description
Main Flowsheet
RCSTR (RCSTR) - Stream Results (Default)
RCSTR (RCSTR)
DS-1
EIN
Mole-Flow Stream=E Substream=MIXED Component=E Units=kmol/hr
View Variables
Edit selected variable
Variable
EIN
Category
All
Blocks
Streams
Model Utility
Property Parameters
Reactions
Reference
Type
Mole-Flow
Stream
E
Substream
MIXED
Component
E
Units
kmol/hr

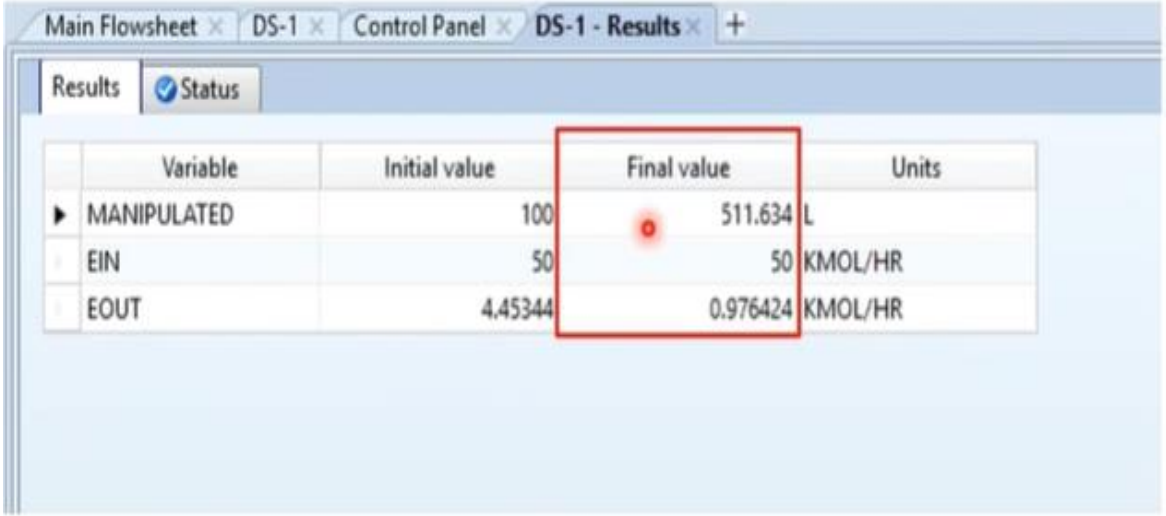




RESULTS AND ANALYSIS:



	Units	B	E	EB
Mass Vapor Fraction		0	1	0
Mass Liquid Fraction		1	0	1
Mass Solid Fraction		0	0	0
Molar Enthalpy	cal/mol	11888	12364.1	9420.5
Mass Enthalpy	cal/gm	152.188	440.73	106.794
Molar Entropy	cal/mol-K	-62.0551	-18.5143	-66.3829
Mass Entropy	cal/gm-K	-0.794421	-0.659956	-0.752538
Molar Density	mol/cc	0.0111405	0.000676172	0.00850761
Mass Density	gm/cc	0.870226	0.0189692	0.750474
Enthalpy Flow	cal/sec	330221	171724	273334
Average MW		78.1136	28.0538	88.212
− Mole Flows	kmol/hr	100	50	104.453
BENZENE	kmol/hr	100	0	54.4534
ETHYLENE	kmol/hr	0	50	4.45344
ETHYL-01	kmol/hr	0	0	45.5466
+ Mole Fractions				
+ Mass Flows	kg/hr	7811.36	1402.69	9214.05
+ Mass Fractions				
Volume Flow	l/min	149.604	1232.43	204.628



Variable	Initial value	Final value	Units
MANIPULATED	100	511.634	L
EIN	50	50	KMOL/HR
EOUT	4.45344	0.976424	KMOL/HR

Sensitivity analysis in Aspen:

Sensitivity analysis in Aspen is a technique used to assess how changes in input variables affect the outputs of a model. It helps in understanding the sensitivity of a process or system, optimizing decisions, and evaluating risks. The process involves defining the objective, selecting input variables, specifying variable ranges, creating the Aspen model, running the sensitivity analysis, analyzing the results, interpreting the findings, and refining the analysis if necessary. It's a valuable tool for making informed decisions and improving process performance.

Thank you