Industrial Processes and Scale-up 2014/2015

Numerical exercize: Simulation of a continuous distillation column

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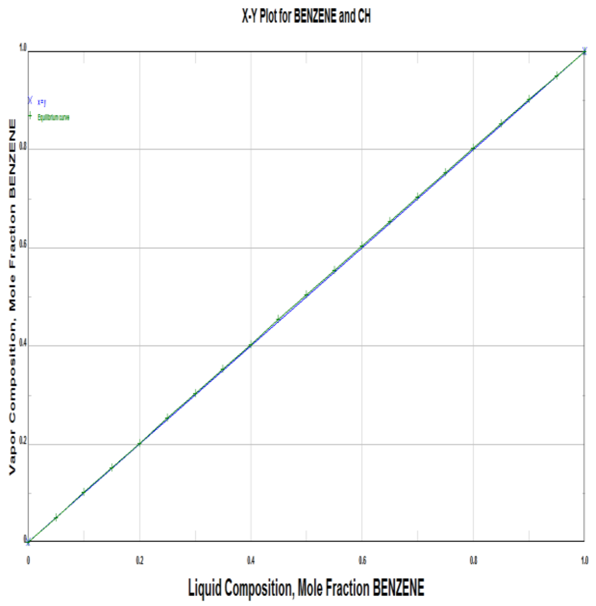
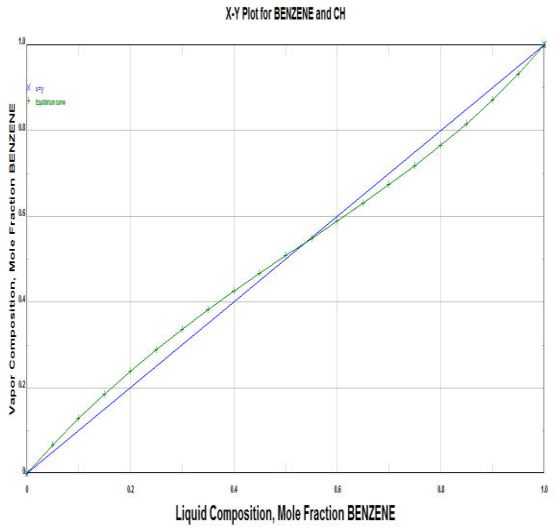
Federico Galli

Cyclohexane-Benzene system: VLE (non ideal) from PRO II database

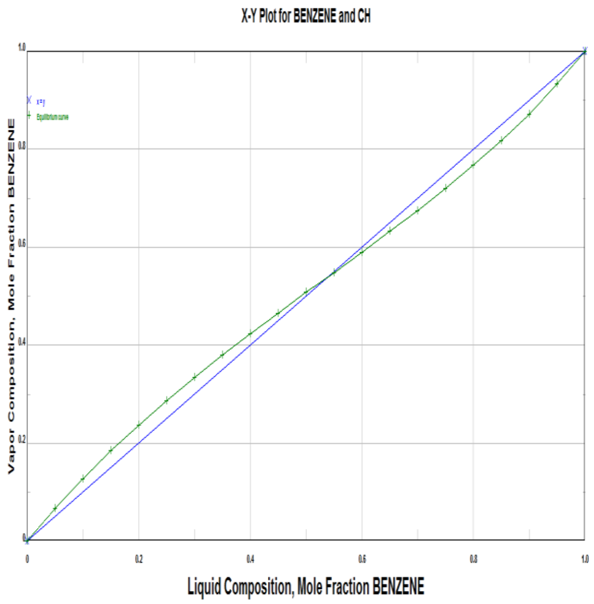
Ideal



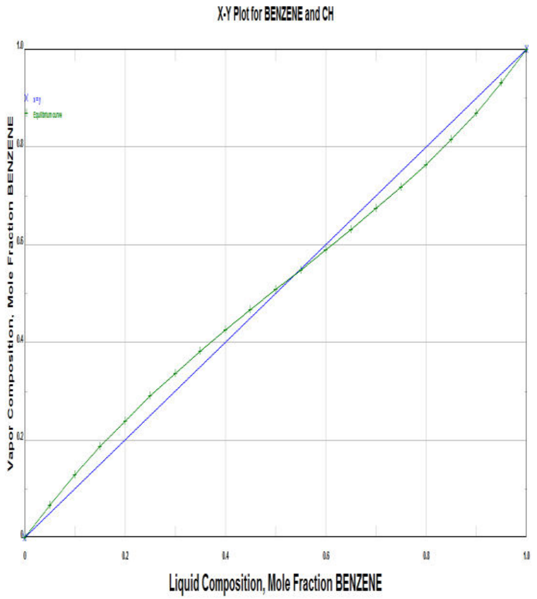
Van Laar



NRTL

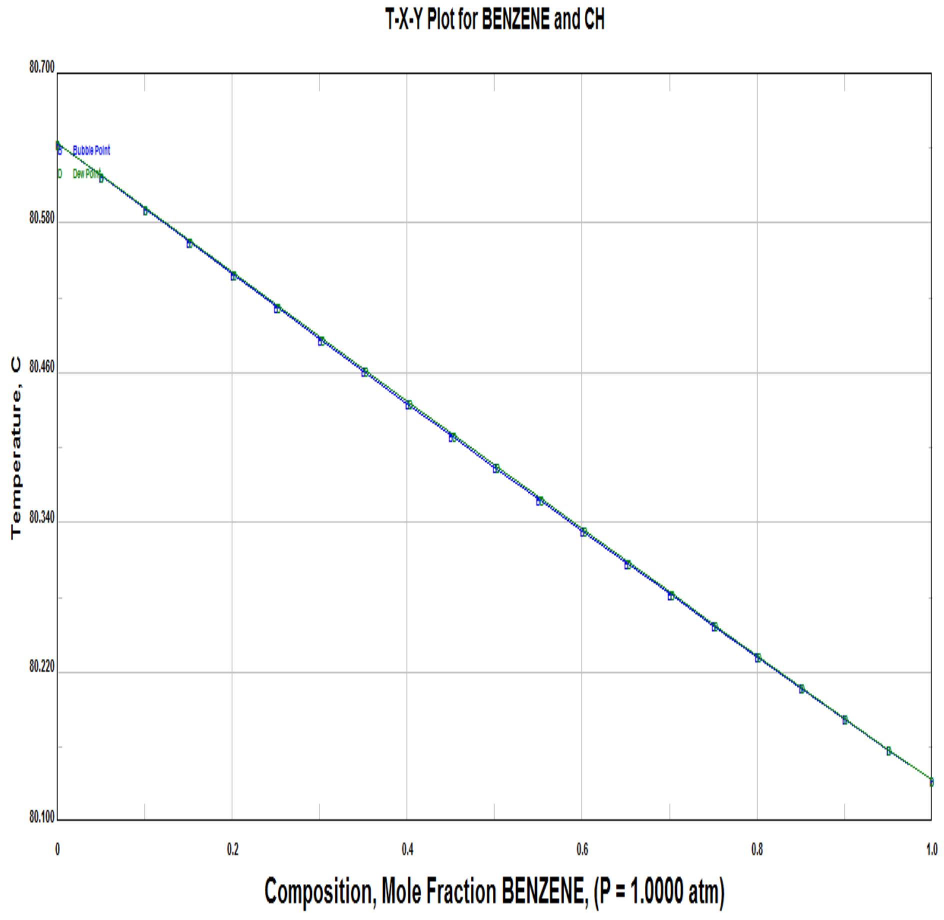


UNIFAC

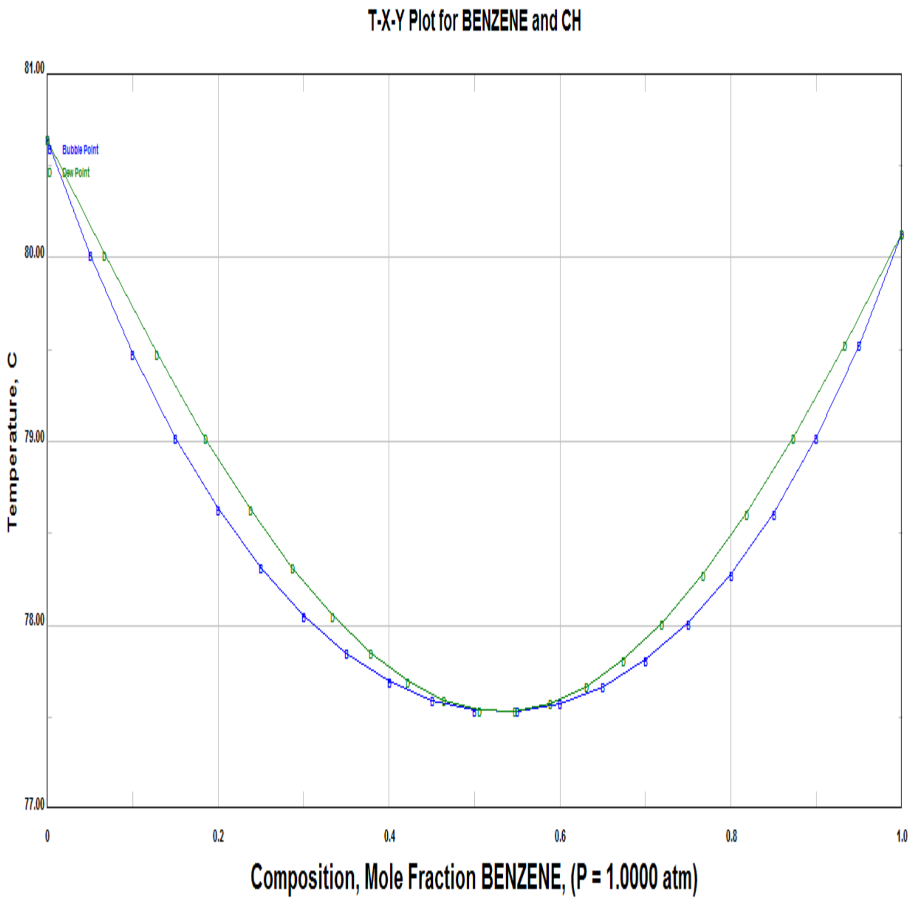


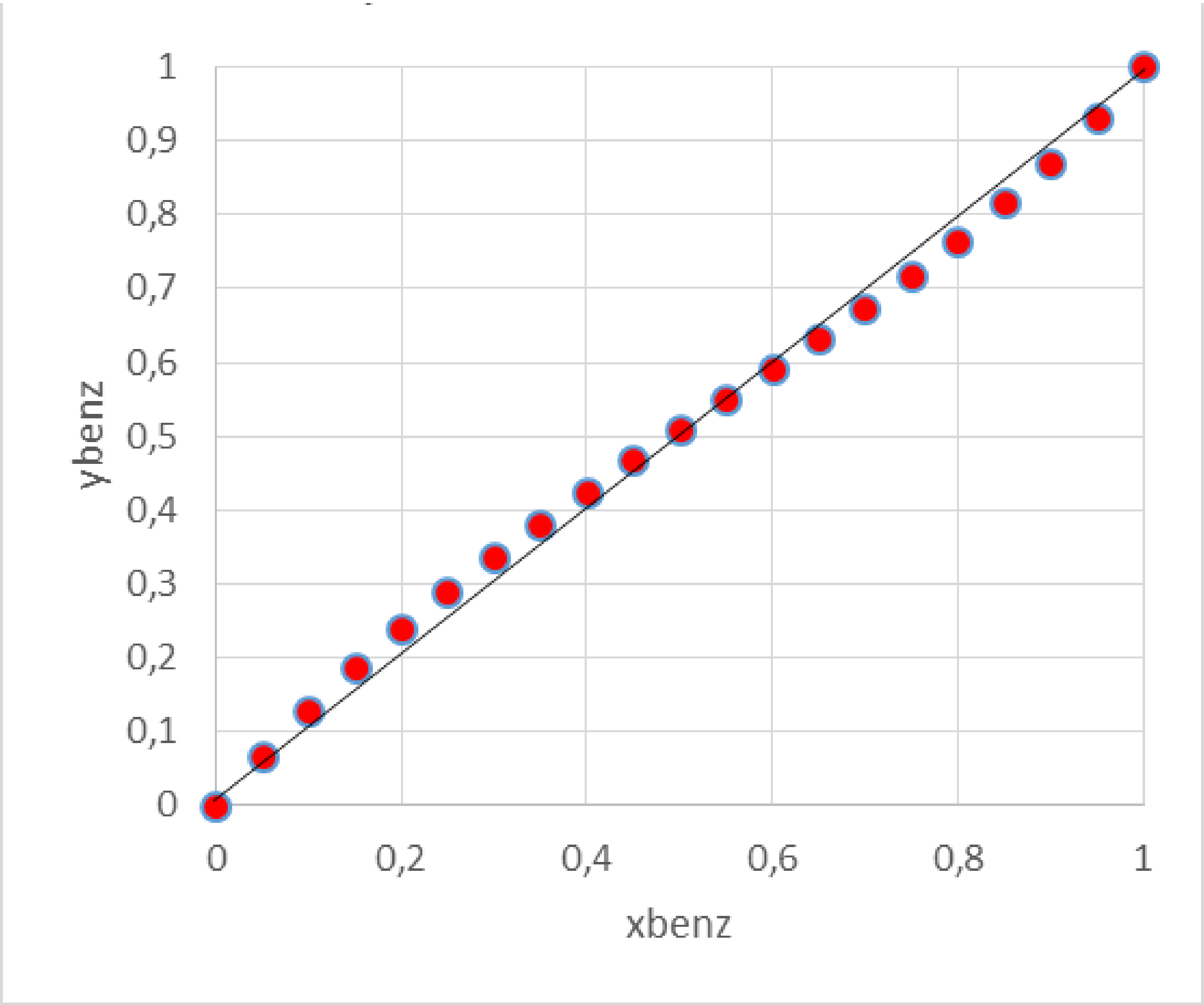
VLE (non ideal) from PRO II database

Ideal



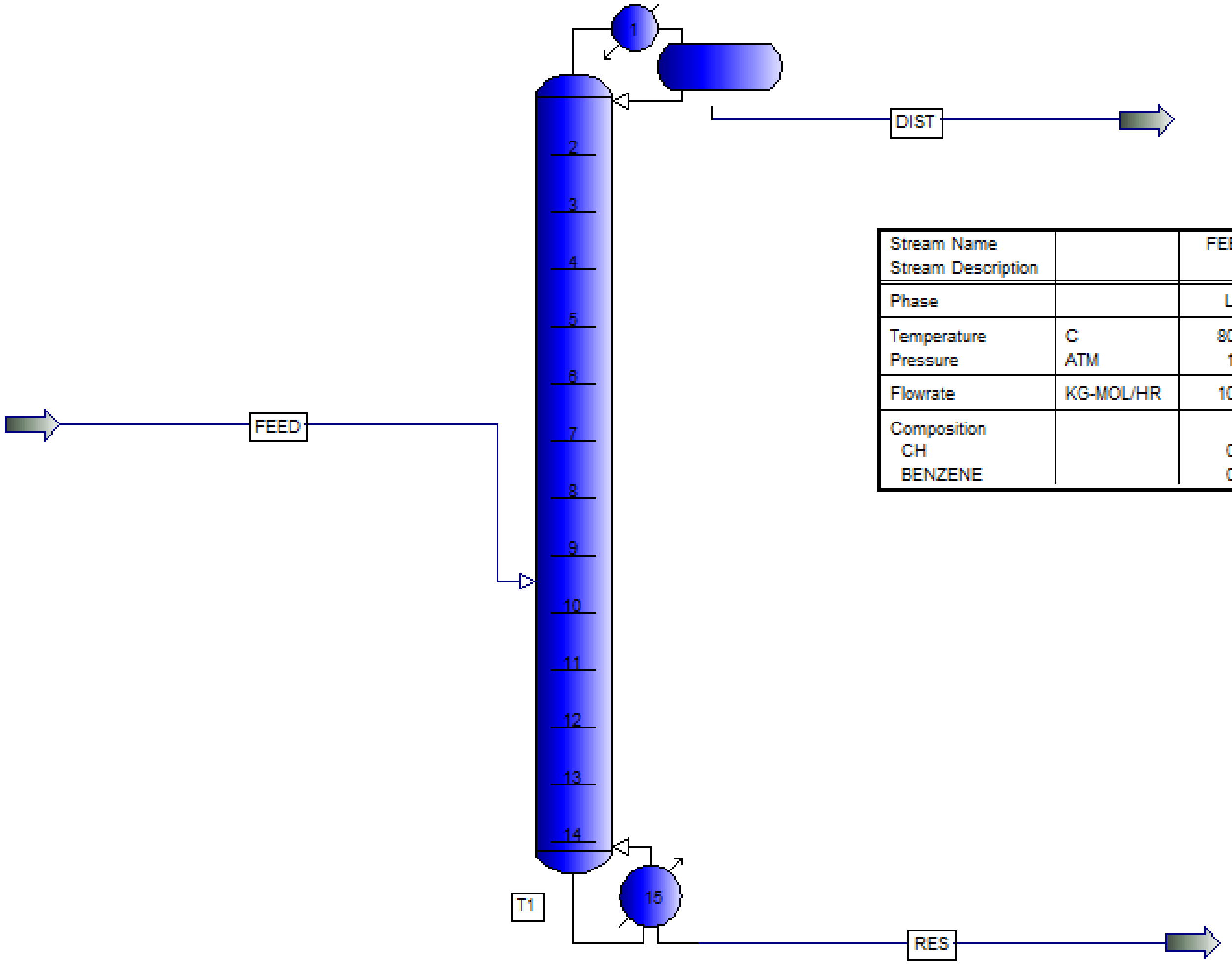
NRTL





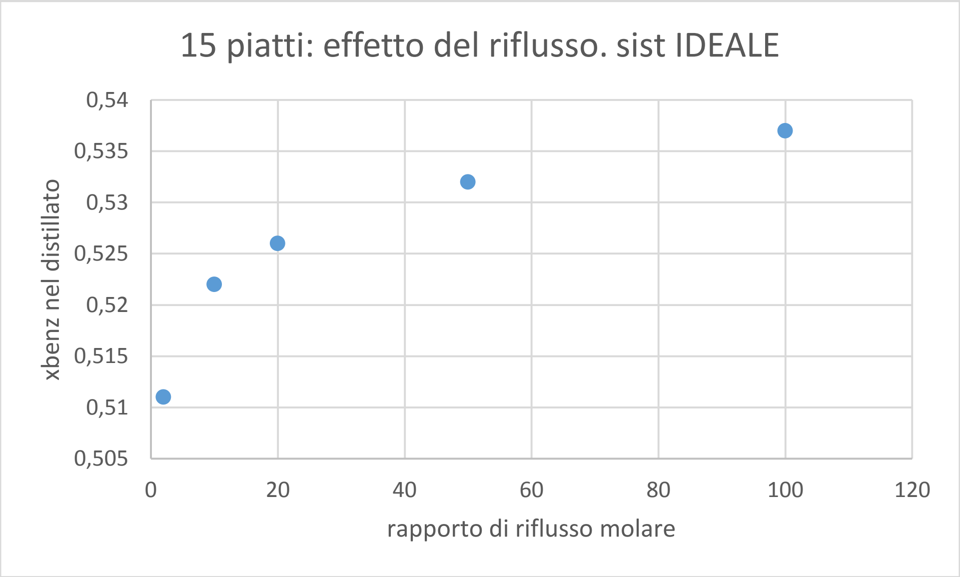
ybenz
xbenz
1
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0
0
0,2
0,4
0,6
0,8
1

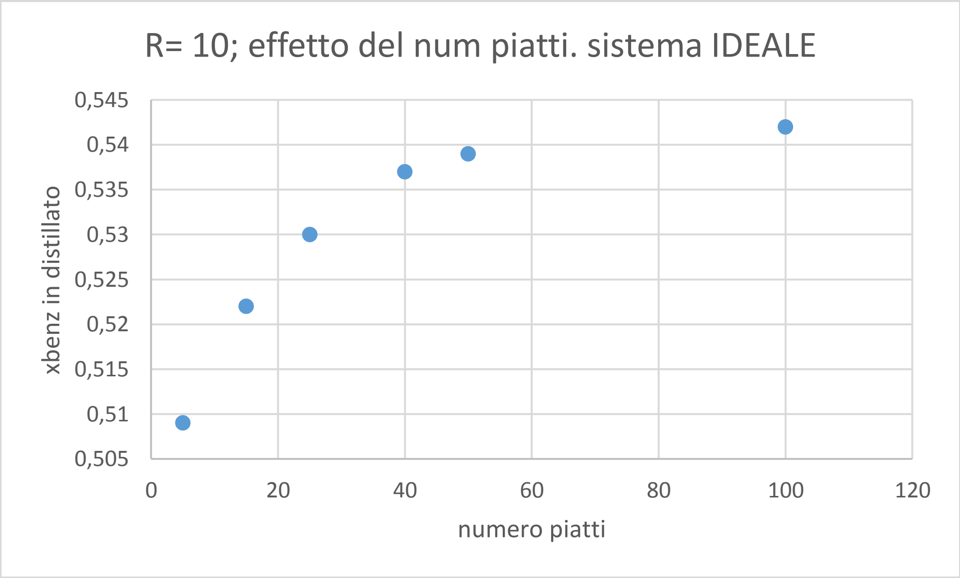
Thermodynamic model: ideal



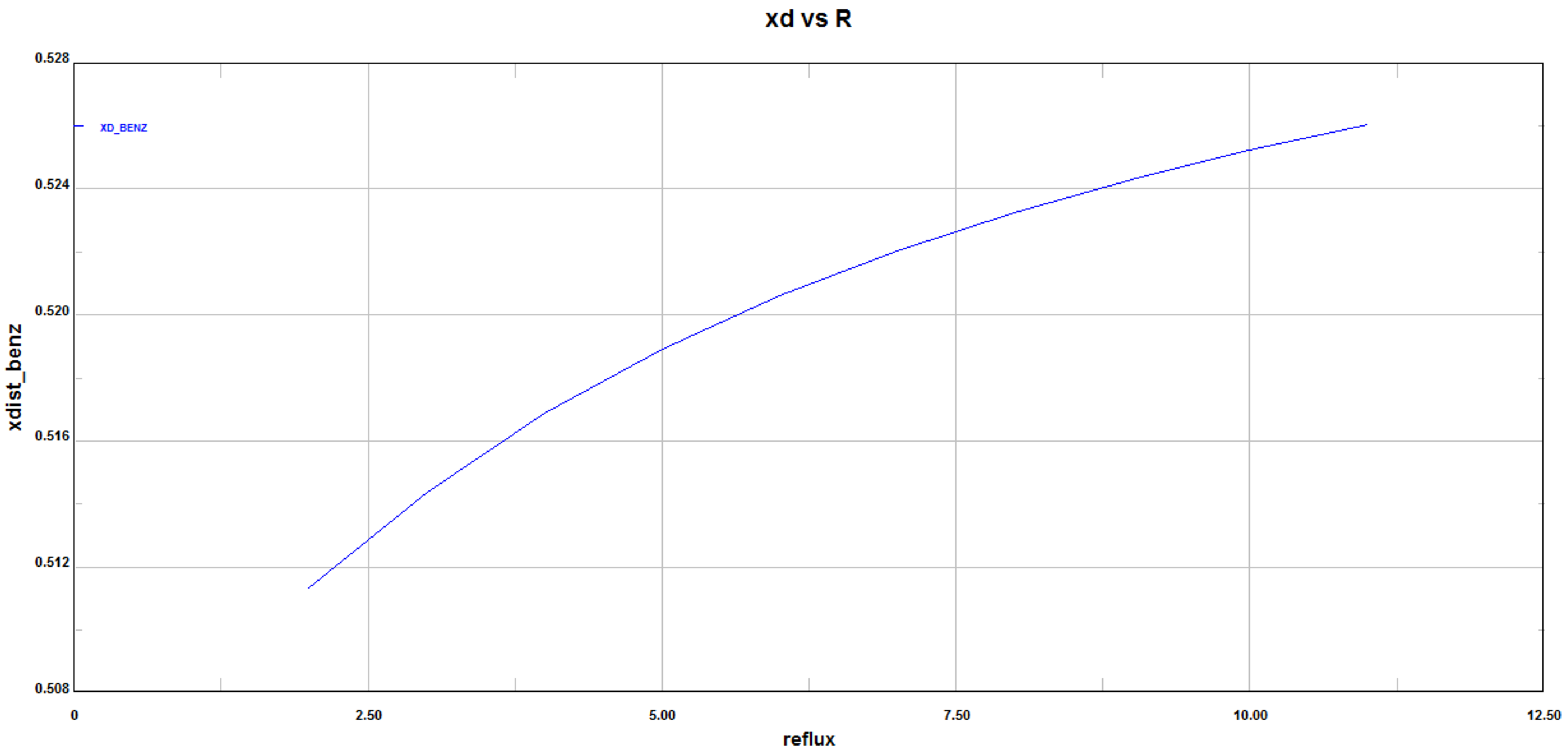
Stream Name Stream Description		FEED	DIST	RES
Phase		Liquid	Liquid	Liquid
Temperature Pressure	C ATM	80,000 1,000	80,365 1,000	80,385 1,000
Flowrate	KG-MOL/HR	10,000	0,400	9,600
Composition CH BENZENE		 0,500 0,500	 0,462 0,538	 0,502 0,498

Results

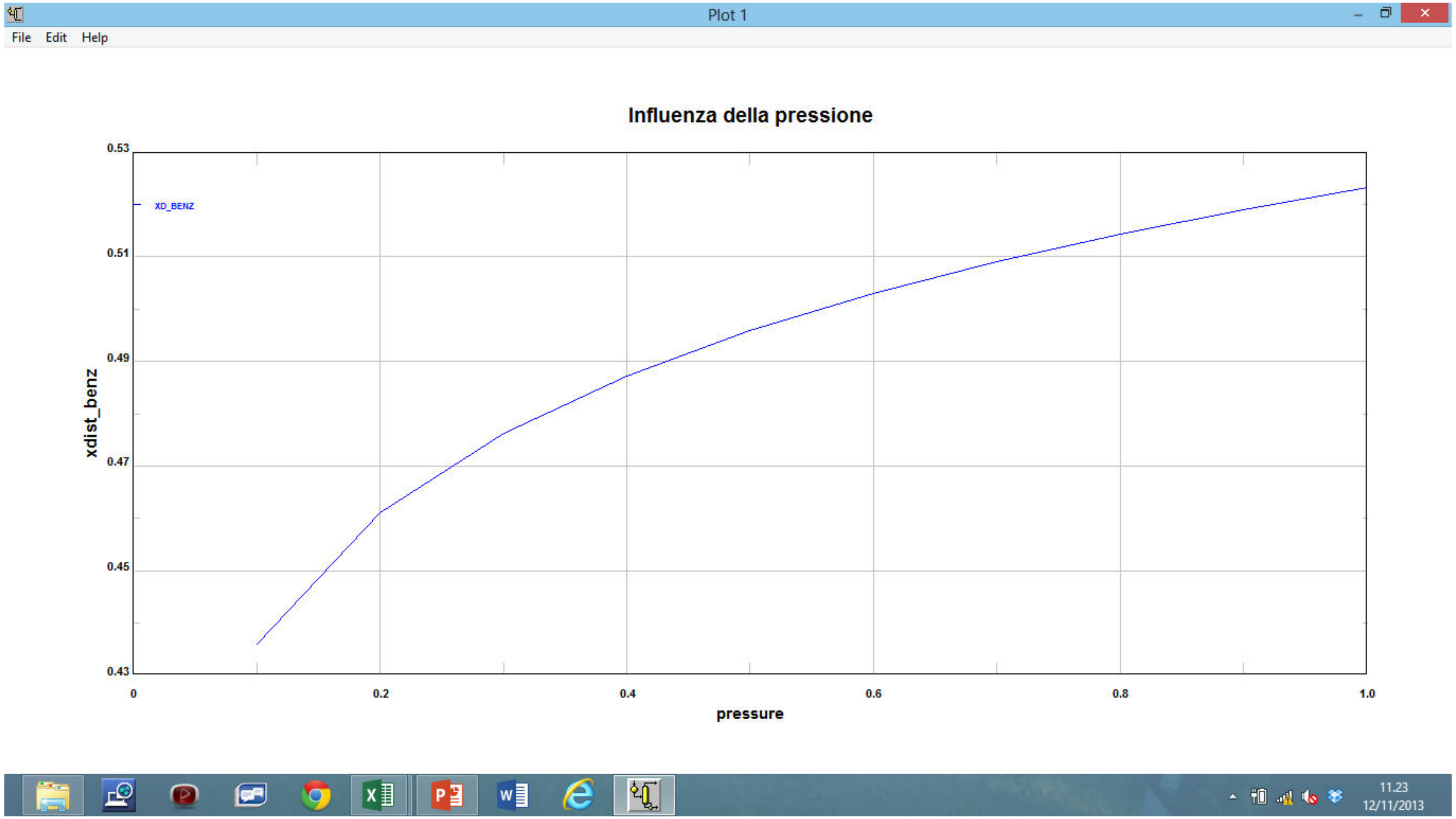

15 piatti: effetto del riflusso. sist IDEALE
xbenz nel distillato
0,54
0,535
0,53
0,525
0,52
0,515
0,51
0,505
0
20
40
60
80
100
120
rapporto di riflusso molare


R= 10; effetto del num piatti. sistema IDEALE
xbenz in distillato
0,545
0,54
0,535
0,53
0,525
0,52
0,515
0,51
0,505
0
20
40
60
80
100
120
numero piatti

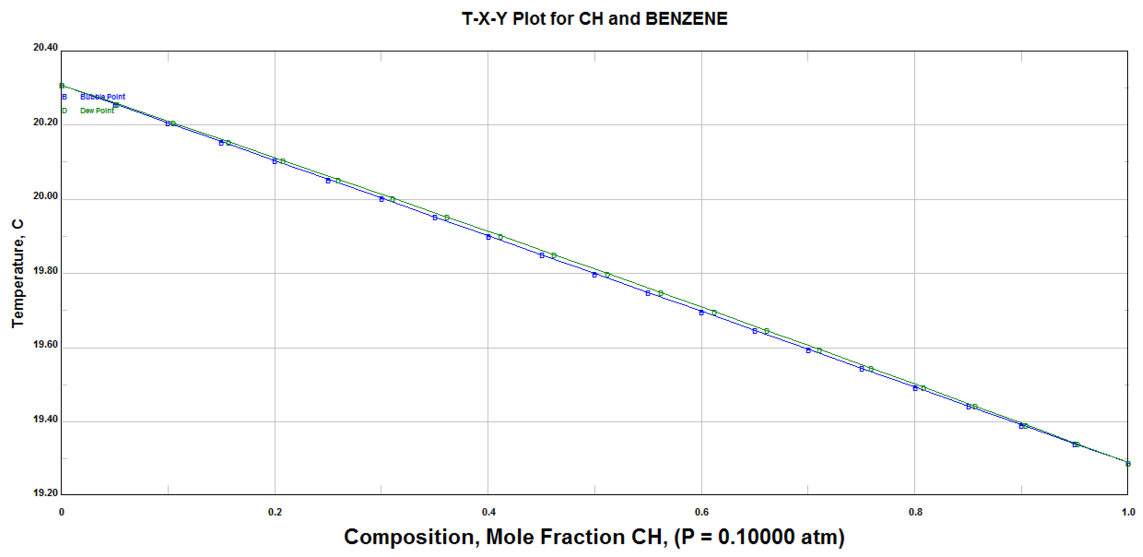
Case study, thermodynamic method ideal
P = 1 atm



Case study, influence of Pressure

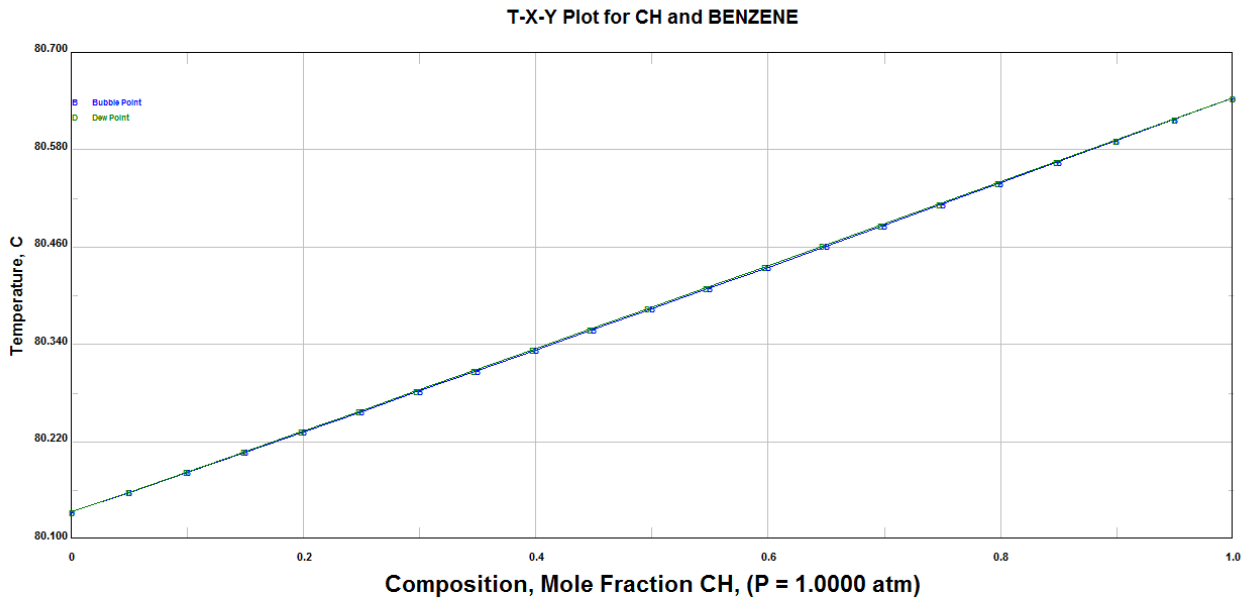


The lower the pressure, the lower the molar fraction of benzene in the distillate, Why?

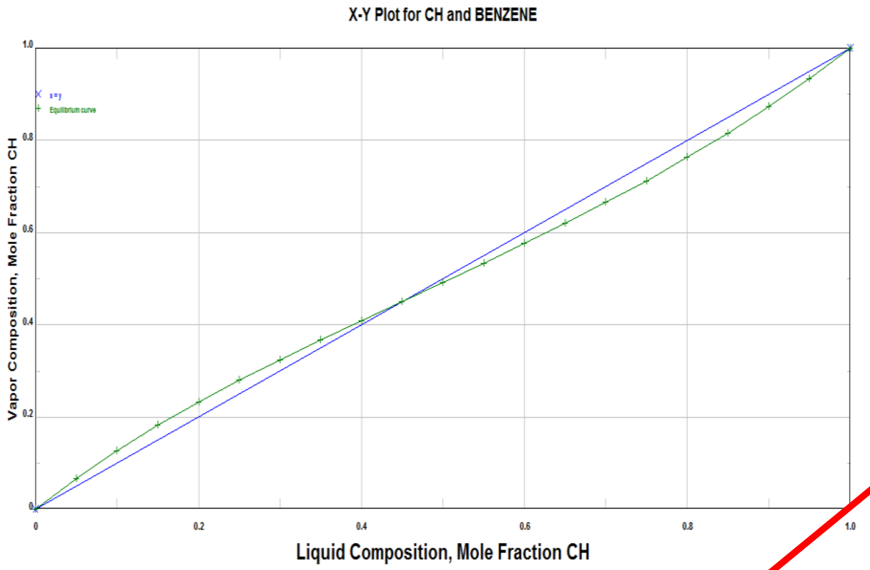


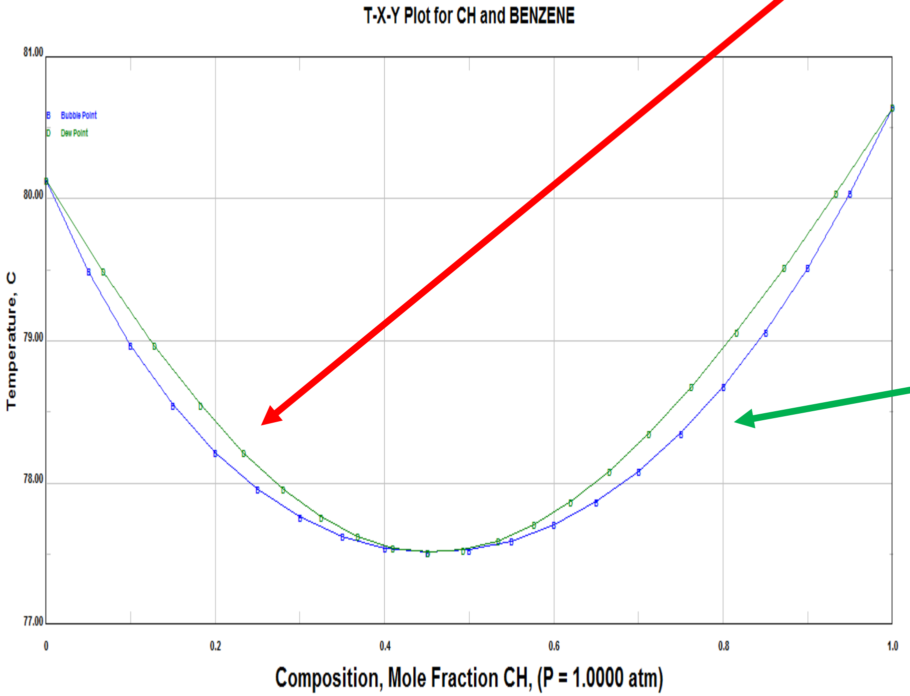
P=0,1 bar

P=1 bar



Same column, thermodynamic model NRTL





Stream Name Stream Description		FEED	DIST	RES
Phase		Vapor	Liquid	Liquid
Temperature Pressure	C ATM	80,000 1,000	77,789 1,000	78,641 1,000
Flowrate	KG-MOL/HR	10,000	4,000	6,000
Composition CH BENZENE		 0,200 0,800	 0,293 0,707	 0,138 0,862

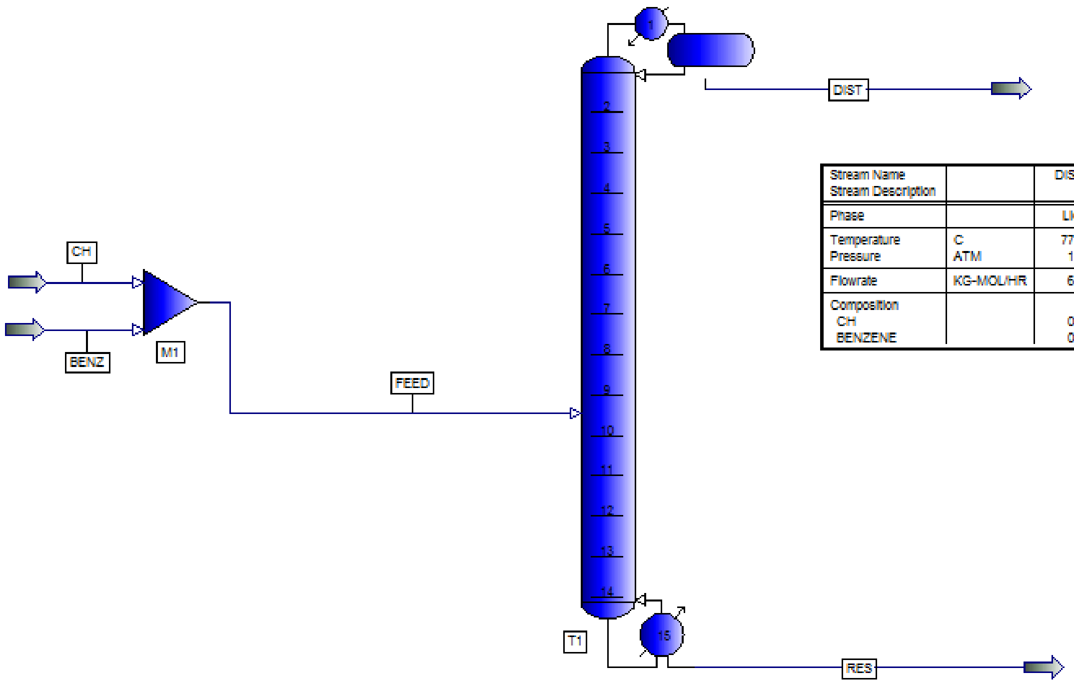
Property Table

Starting from the left of the azeotrope, I will have a distillate rich in CH

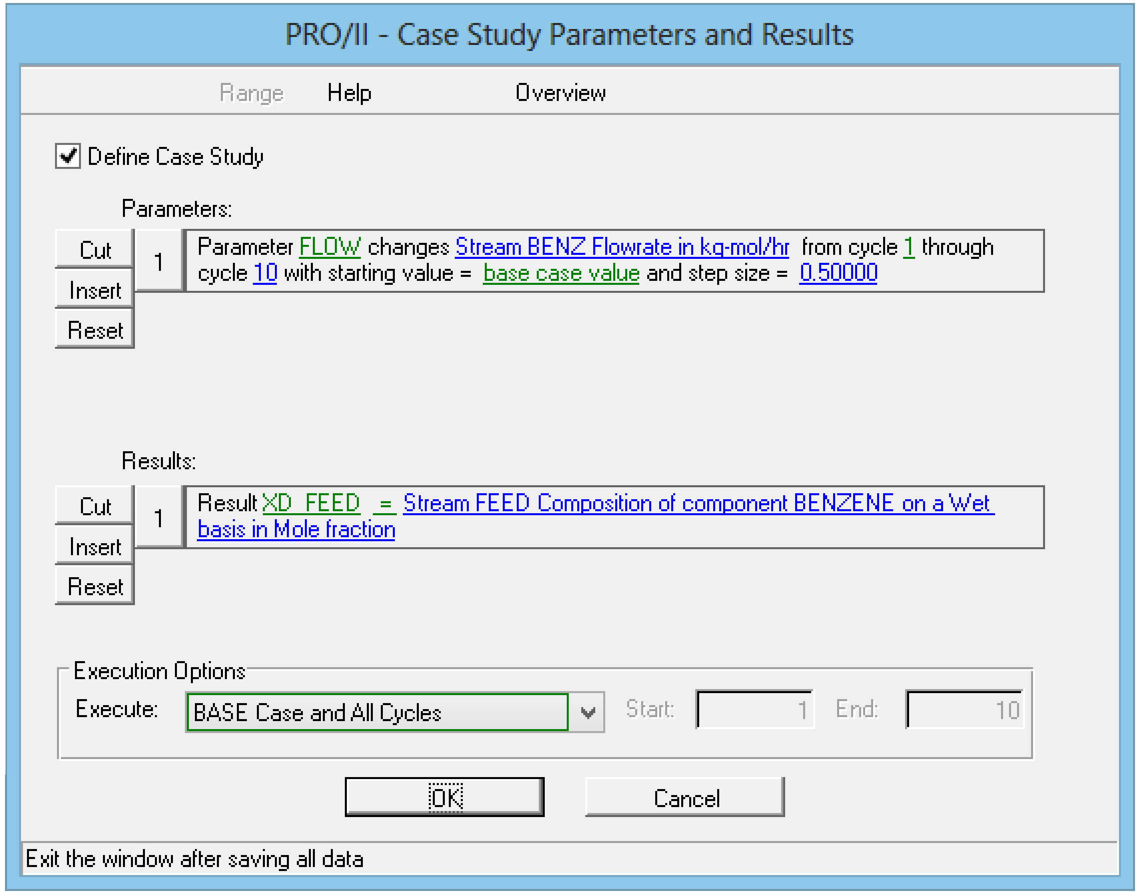
Stream Name Stream Description		FEED	DIST	RES
Phase		Vapor	Liquid	Liquid
Temperature Pressure	C ATM	80,000 1,000	78,075 1,000	79,221 1,000
Flowrate	KG-MOL/HR	10,000	4,000	6,000
Composition CH BENZENE		 0,800 0,200	 0,698 0,302	 0,868 0,132

Starting from the right of the azeotrope, I will have a distillate rich in B

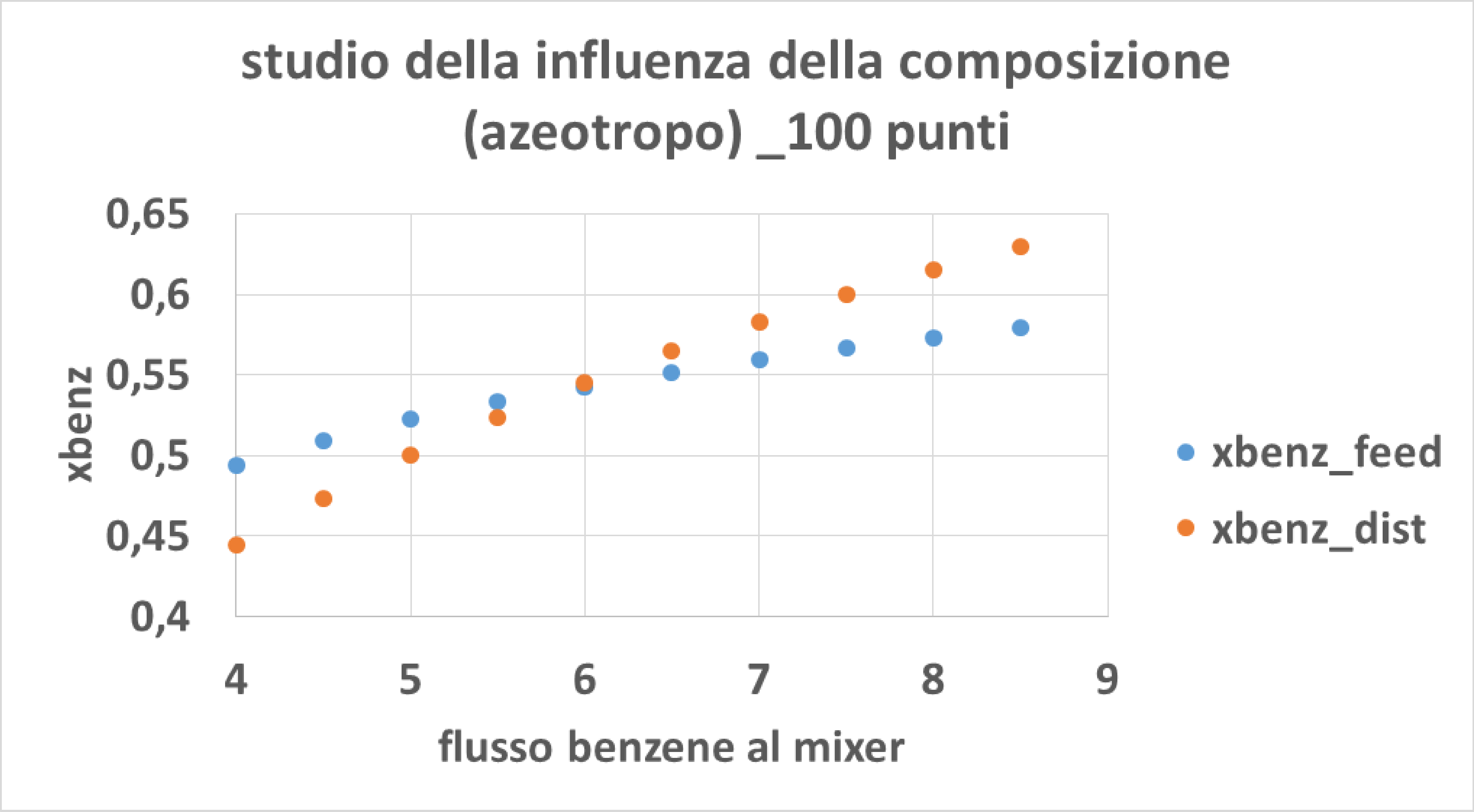
Case Study , different feed composition

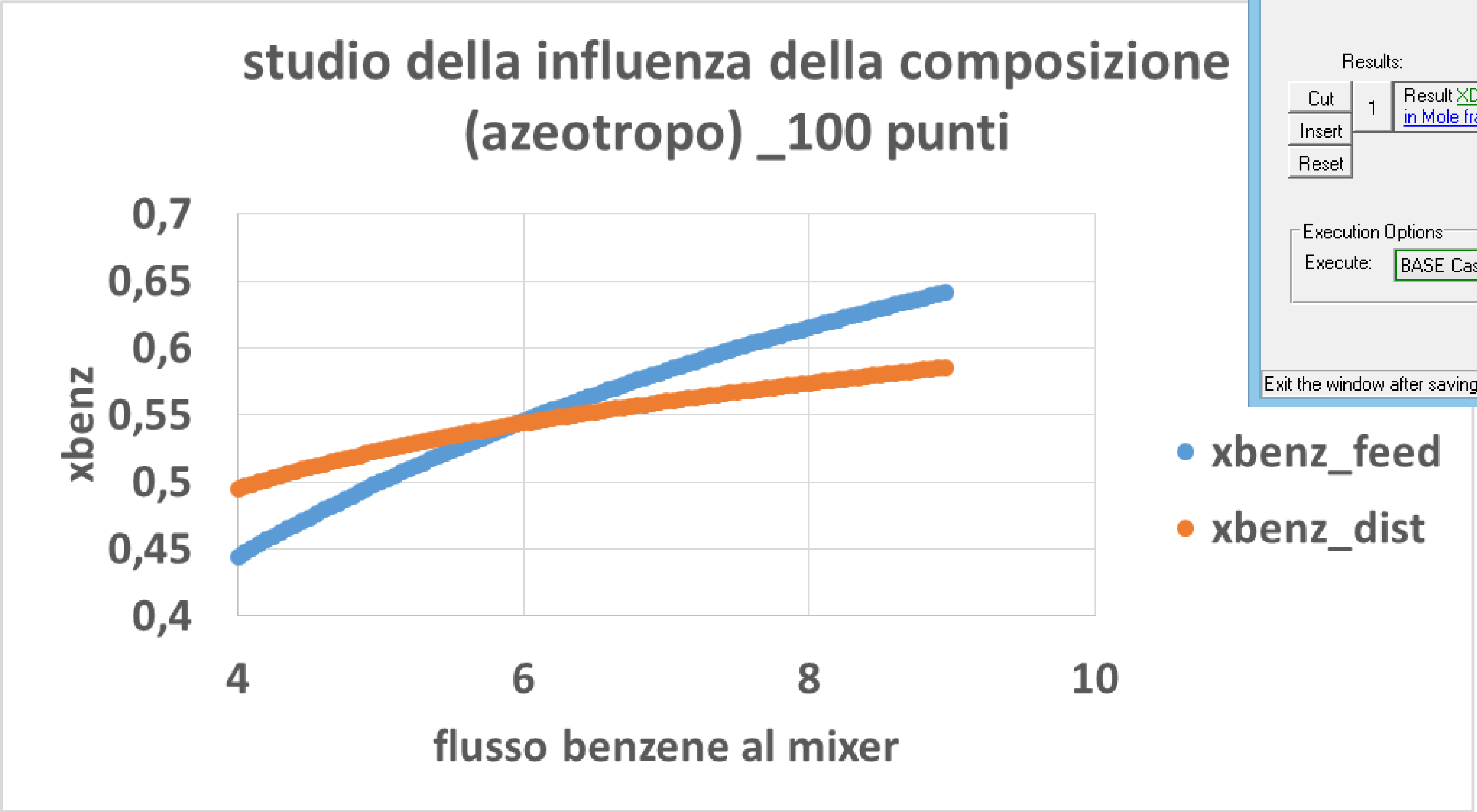


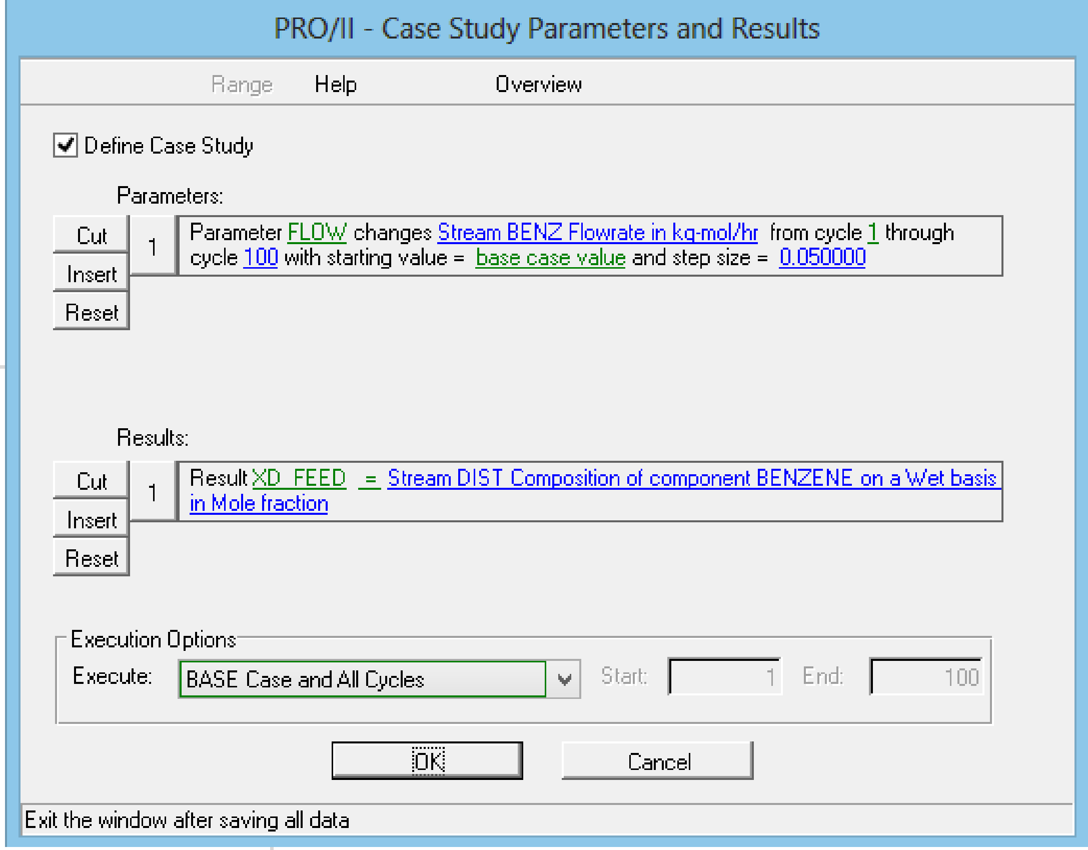
Stream Name Stream Description		DIST	RES	FEED
Phase		Liquid	Liquid	Mixed
Temperature Pressure	C ATM	77,536 1,000	77,894 1,000	77,607 1,000
Flowrate	KG-MOL/HR	6,000	3,000	9,000
Composition CH BENZENE		 0,505 0,495	 0,656 0,344	 0,556 0,444

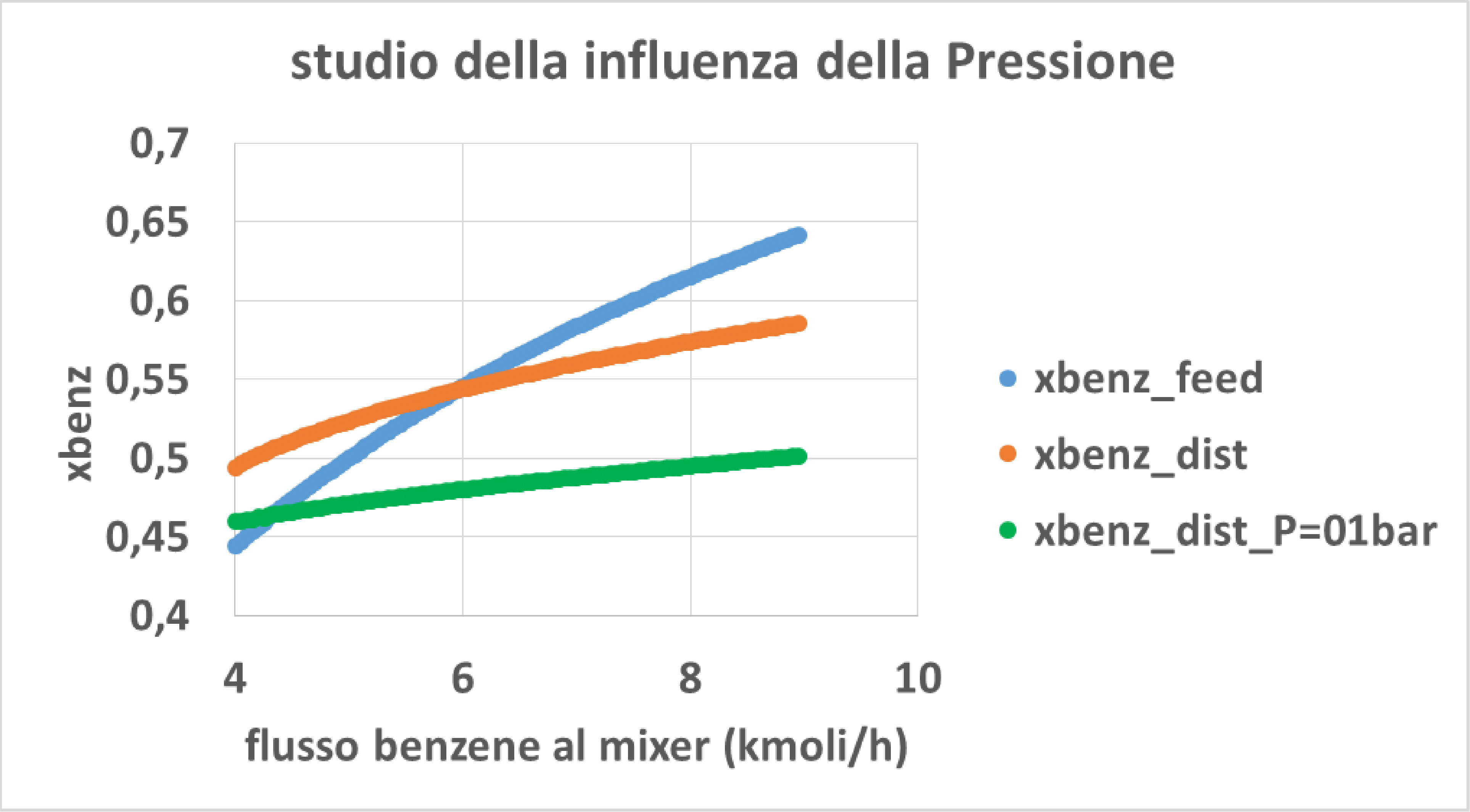


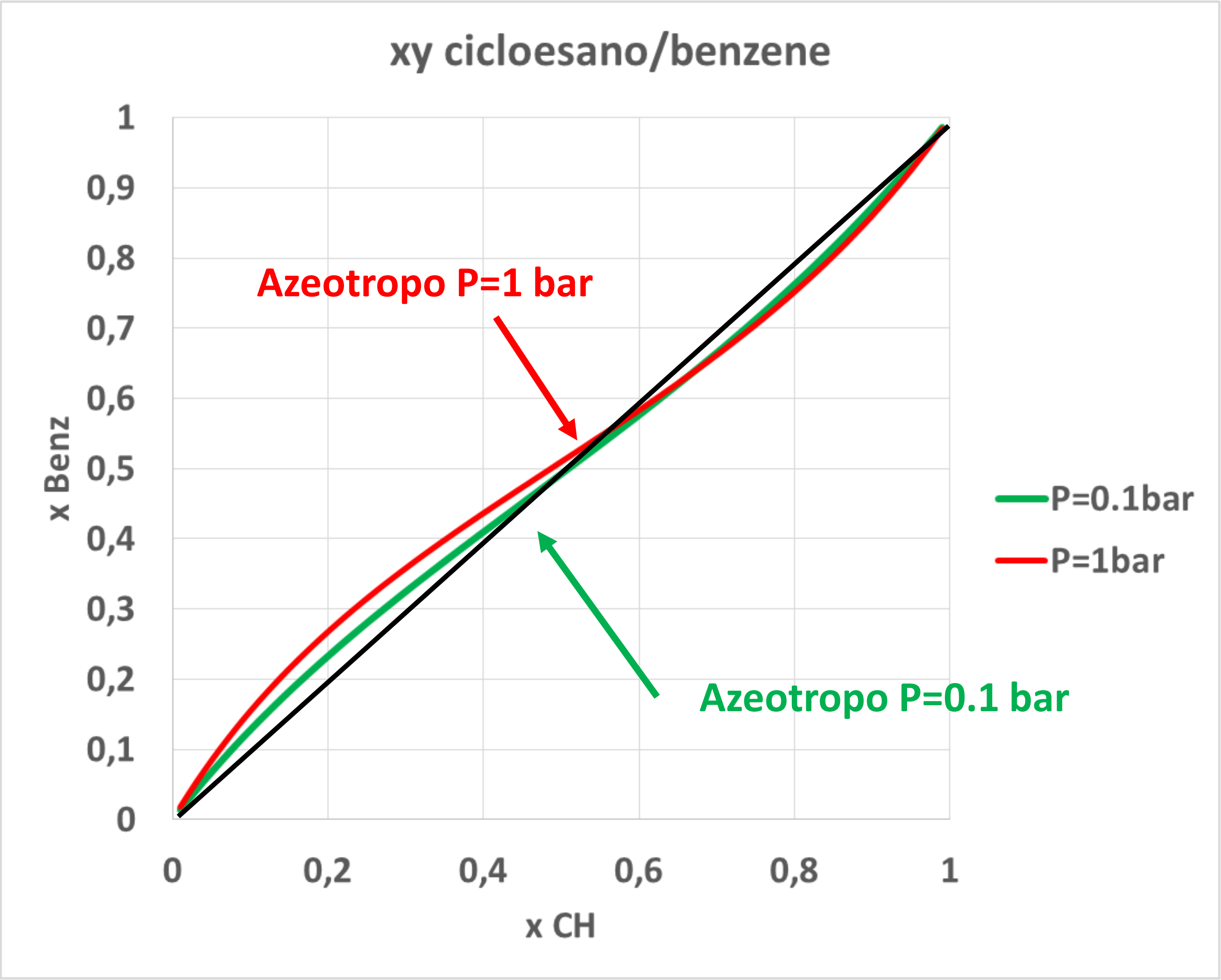
Watch out the mass balances!!!! The flowrate fed (for every case study) must meet the column specifications!. This case starts from 5+4 mkoli/h and ends at 5+9 kmoli/h. It was set a pecification of D= 6kmol/h. Another way is to vary the specification, for example set a composition, but this one could be more restrictive


studio della influenza della composizione (azeotropo) _100 punti
0,65
0,6
0,55
0,5
0,45
0,4
xbenz
4
5
6
7
8
9
flusso benzene al mixer
xbenz_feed
xbenz_dist


studio della influenza della composizione (azeotropo) _100 punti
0,7
0,65
0,6
0,55
0,5
0,45
0,4
xbenz
4
6
8
10
flusso benzene al mixer
xbenz_feed
xbenz_dist


PRO/II - Case Study Parameters and Results
Range
Help
Overview
Define Case Study
Parameters:
Cut
Insert
Reset
1
Parameter FLOW changes Stream BENZ Flowrate in kg-mol/hr from cycle 1 through cycle 100 with starting value = base case value and step size = 0.050000
Results:
Cut
Insert
Reset
1
Result XD_FEED = Stream DIST Composition of component BENZENE on a Wet basis in Mole fraction
Execution Options
Execute:
BASE Case and All Cycles
Start:
1
End:
100
OK
Cancel
Exit the window after saving all data


studio della influenza della Pressione
0,7
0,65
0,6
0,55
0,5
0,45
0,4
xbenz
4
6
8
10
flusso benzene al mixer (kmoli/h)
xbenz_feed
xbenz_dist
xbenz_dist_P=01bar

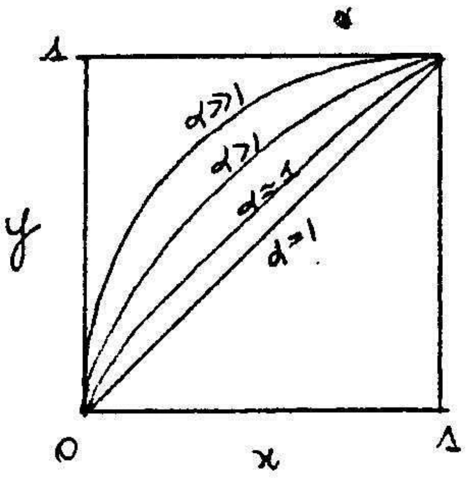


xy cicloesano/benzene
Azeotropo P=1 bar
Azeotropo P=0.1 bar
x Benz
x CH
0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1
0
0,2
0,4
0,6
0,8
1
P=0.1bar
P=1bar

Other important industrial systems on which you can exercise:

1) Water/ethanol
2) Water/acetic acid
3) Water/acetic acid/p-xylene
4) Toluene/isooctane/phenol

If the relative volatility is equal to 1, the equilibrium curve is the diagonal x=y, instead if alfa is high, the number of theoretical stages is low



Remember the 5 different cases in the VLE!

In the second case we will have:

$$\alpha_{ij} = \frac{\gamma_i p_i^0(T)}{\gamma_j p_j^0(T)}$$

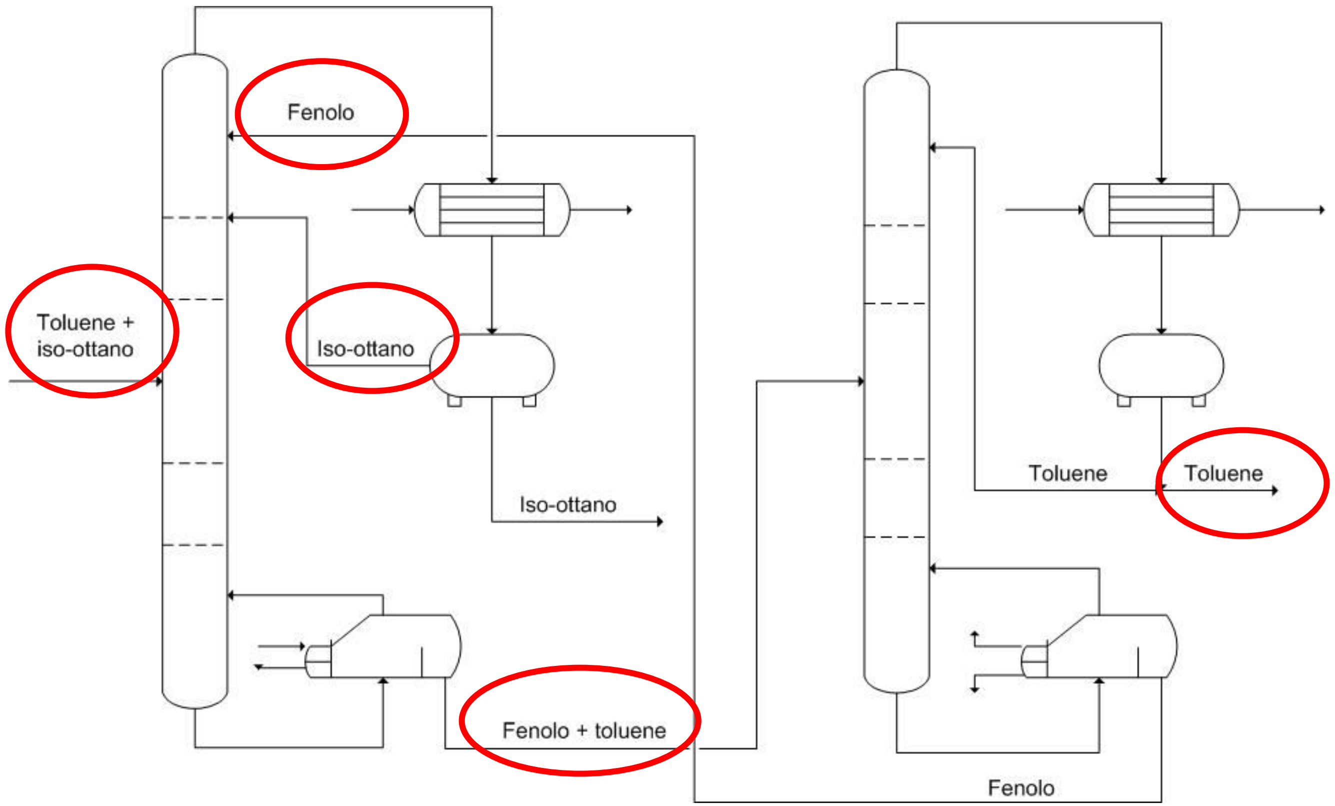
If the relative volatility is close to 1, I can introduce a third component called ENTRAINER, which interacts with one of the two components in such a way to increase the value of alfa, by altering the activity coefficients.

The drawback is that the system is now composed of three components.

The characteristics a good entreiner should have are here reported:

1. High selectivity, in order to make easier the separation using the less amount of entrainer possible.
2. Easier separation from the mixture to which is added. Also the entrainer should not form azeotropes with both the original components. Usually an entrainer with a higher boiling point compared with the ones of the main components is used.
3. It should possess good chemical (stability, corrosion), physical (viscosity) and economical.

A good example: TOLUENE (111°C)/ISOOCTANE (99°C), in which PHENOL (181°C) is used as entrainer



Il solvente viene alimentato in testa alla prima colonna in modo tale da averlo in alta concentrazione su tutta la colonna. Esce dal fondo con il componente meno volatile

T eb toluene= 110°C
T eb isoottano = 99.3°C
T eb fenolo= 181.4°C

In testa alla prima colonna si ottiene isottano praticamente puro e in coda una miscela di fenolo + toluene che viene separata nella seconda colonna, in coda alla quale si ottiene il fenolo che viene riciclato nella prima colonna.