THE NEW APPROACH TO ISOPROPYLBENZENE DISTILLATION FLOWSHEET SYNTHESES IN PHENOL-ACETONE PRODUCTION

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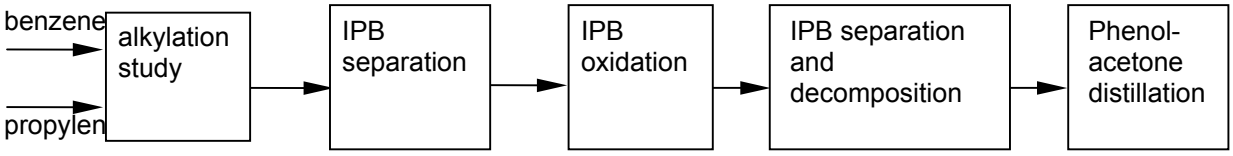
DESCRIPTION OF THE PROCESS

There exist several methods of phenol-acetone production. In our case we used material balance of alkylation mass obtained by method of combined production of phenol and acetone with aluminum chlorate as the base of catalyst complex according to the technology created by P.G. Sergeev, R.U.Udris, B.D.Krugalov and M.S.Nemtsov in 1949 [1].

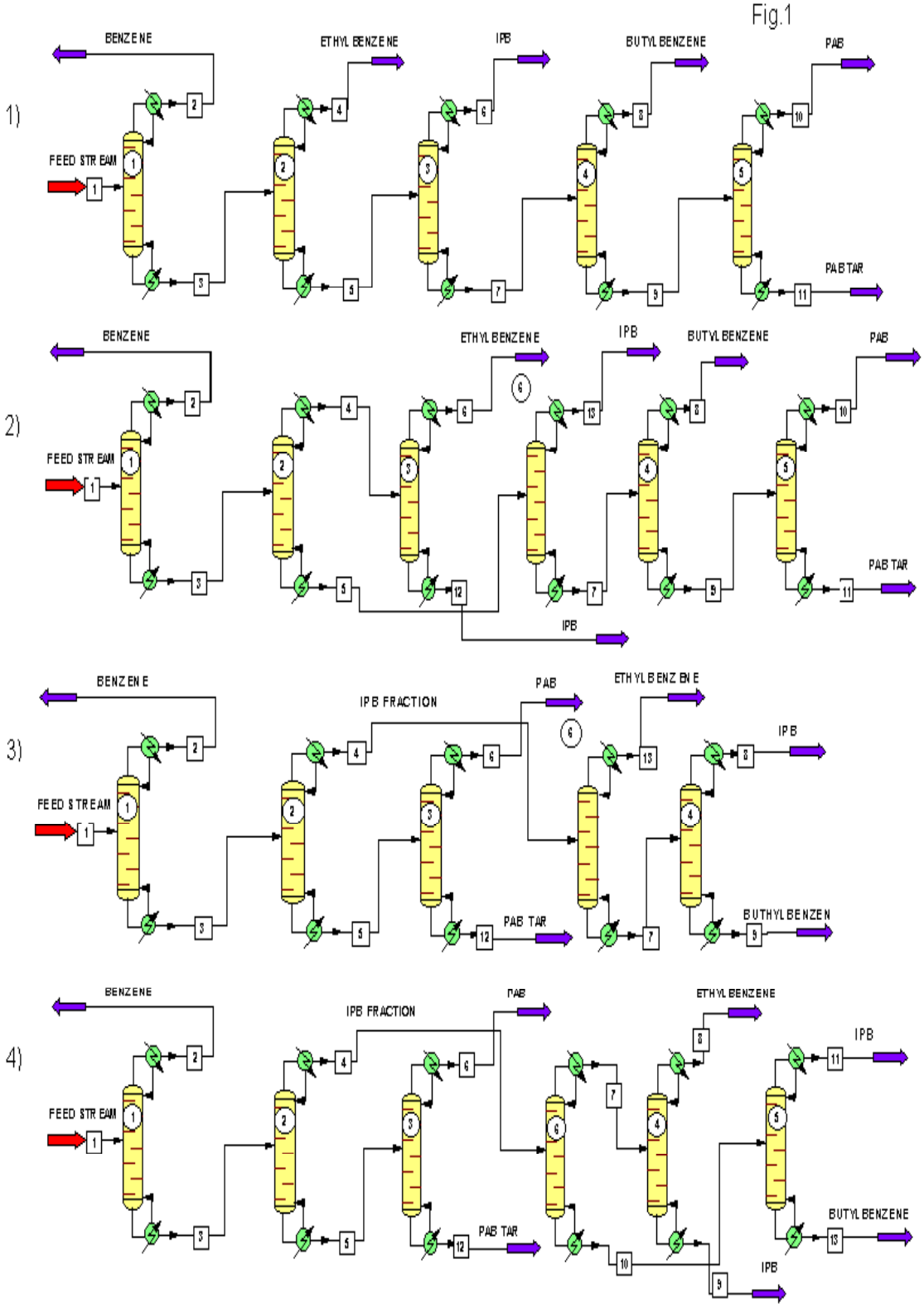
In Russia there are several plants by this technology with some different modifications and production capacity. The train of such production is shown below.



In the chain of isopropylbenzene-IPB separation the reaction mass after series of intermediate tanks and absorber, used for decanting heavy catalysts complex and removing obtained gases (propane - inert for this case of reaction), proceeds to distillation stage. Depending on operating factors, such as propylene/benzene ratio, temperature of alkylation, residence time contact, pressure differentials, feed stock quality (for example - propane contents in propylene), concentration of catalysts in reactor, etc., possible variations in reaction mass composition. The average composition of alkylation product is as follows: circa 50% by wt. benzene, 30-35% by wt. isopropylbenzene, 15-18% by wt. of polyalkylbenzenes - PAB (mainly *m*- and *p*-diisopropylbenzenes), 0.2% by wt. of water. As mentioned above the composition is affected by impurities in feed stock, so if the propylene contents ethylene and butenes having also participation in reaction with benzene, the some ethylbenzene and butylbenzenes will be present [1]. One of the byproducts is polyalkylbenzenes tar, which is actually a mixture of heavier alkyl-aromatics: tetraalkylbenzenes 20-40% by wt., alkyltetrapenes 15-35% by wt., alkylphenilpropanes 25-45% by wt. The catalyst used affects PAB isomeric structure. In our case, the catalyst (aluminum chlorate complex) results in the following PAB fraction composition: 70-73% by wt. *m*-diisopropylbenzene, 25-30% by wt. *p*-diisopropylbenzene, *o*- diisopropylbenzene practically absent [1].

The existing distillation stage of IPB may be arranged in 4 general options:

Fig.1



The third type of flowsheet (Fig.1) was used as the base for distillation calculation, because actual industrial data were available for only mentioned type of flowsheet.

The actual production of a plant was used as the base for investigation of distillation flowsheet. According to the actual data, the ratio of components for feed and product streams are the following (Tab.1, 2):

Tab.1 The actual industrial data of feed stream

Flowrates	kg/h	weight %
Benzene	31 977,90	49,71%
Toluene	133,30	0,21%
Ethylbenzene	739,30	1,15%
Isopropylbenzene	19 722,70	30,66%
n-propylbenzene	42,20	0,07%
Tert-Butylbenzene	12,90	0,02%
Sec-Butylbenzene	154,40	0,24%
Cymenes	61,90	0,10%
N-Butylbenzene	14,30	0,02%
Diisopropylbenzenes	9 752,50	15,16%
ThriisopropylBenzenes	748,10	1,16%
Polyalkylbenzene Tar	965,70	1,50%
Total	**64 325,20**	**100,00%**

Tab.2 The actual industrial data of product streams

Components	PAB	PAB tar	Ethyl Benz	IPB	Sec-butyl Benz
	%, weight	%, weight	%, weight	%, weight	%, weight
Benzene	0	0	0,0509	0	0
Toluene	0	0	0,0162	0,0011	0
Ethylbenzene	0	0	0,8306	0,0016	0
Isopropylbenzene	0,0091	0	0,1023	0,9968	0
n-propylbenzene	0	0	0	0,0003	0,115
Tert-Butylbenzene	0	0	0	0,0001	0,0338
Sec-Butylbenzene	0	0	0	0,0001	0,4705
Cymenes	0	0	0	0	0,1903
N-Butylbenzene	0	0	0	0	0,044
Diisopropylbenzenes	0,9116	0,1613	0	0	0,1464
ThriisopropylBenzenes	0,065	0,0645	0	0	0
Polyalkylbenzene Tar	0,0143	0,7742	0	0	0

For calculation reasons the above composition was arranged into the following: (Tab.3):

Tab. 3 The feed stream composition is used for simulation

Flowrates	kg/h	Weight %	M weight	Normal boiling T
Benzene	31 977,9	49,71%	78,114	80,09
Ethylbenzene	739,3	1,15%	106,167	136,20
Isopropylbenzene	19 722,7	30,66%	120,174	152,41
Sec-Butylbenzene	243,5	0,38%	134,221	173,33
M-DiisopropylBz	10 500,6	16,32%	162,270	203,18
23-2C1-23-2PhnC4	965,7	1,50%	238,373	315,85
Toluene	133,3	0,21%	92,141	110,63
N-Propylbenzene	42,2	0,07%	120,194	159,24
Water	0,0	0,00%	18,015	100,00
Total	**64 325,12**	**100,00%**		

Stream temperature	deg C	80
Pressure	atm	1,936
Mass flowrate	kg/h	64 325,12
Actual vol	m3/h	79,202

The amount of M-DiisopropylBz is increased by ThriisopropylBenzenes due to in actual balance the main part of ThriisopropylBenzenes (91% wt.) come to PAB fraction as recycle stream. In fact, ThriisopropylBenzenes are already PAB group components, that cannot to be transalkylated [1], but are united with M-DiisopropylBenzene to simulate close-to-actual heat and material balance. As shown above PAB tar is a fraction that consists of a great number of components. To simplify calculations the number of these components is reduced to the use of 2,3-dimethil-2, 3-diphenilbutane (2,3-2C1-2,3-2PhnC4) alone.

PURPOSE OF THE INVESTIGATION

Isopropylbenzene (IPB) distillation stage in phenol-acetone synthesis was used as the subject for the new flowsheet development method. The proposed sequence of the flowsheet investigation offered to revise the operating production by engineers of the plant for reducing of operating costs (mainly energy saving). The following chain of flowsheet syntheses was been carried out to reach the aim:

- ✓ Analysis of the actual production and choice of simulation mode (section 3 of the article)
- ✓ Flowsheet synthesis by adding water as a polar agent (section 4 of the article)
- ✓ Heat recuperation by applying elements of Pinch analysis (section 5 of the article)

ANALYSIS OF REAL PRODUCTION AND CHOICE OF SIMULATION MODE

Phase equilibrium model

The Soave-Redlich-Kwong model has been chosen to calculate the existing mixture distillation. The Soave-Redlich-Kwong (SRK) equation is very effective to predict K-values for hydrocarbon systems at medium to high pressures. Good results have been obtained by using this method for demethanizers, de-ethanizers, depropanizers, debutanizers, etc. The compressibility and mixture fugacity coefficients for both vapor and liquid phases are derived from the Soave-Redlich-Kwong equation of state.

Developing models of industrial columns by rigorous mass-transfer calculation

The best way is to use the mass transfer model for each distillation simulation with obligatory column geometry.
The calculations used:
Correlation of number of transfer units AIChE (1958), Chan and Fair (1985)
Correlation of transfer NTU to mass transfer coefficients - Bennett (1983)
Correlation of mass transfer coefficients Zuiderweg (1982) [3]

Mass transfer model is to be used only with reliable industrial sizing data of the bubble cap trays for each of the 6 columns in the calculated flowsheet (Fig.2, section 3.3). Otherwise the result of simulation will be calculated incorrect. We can draw as an example the Tab. 4, 7, 10 of calculated mass-transfer coefficients of column K 22 as the matrix for each component for three points - top, bottom and medium trays and corresponding values of overall number of transfer units (NTU) Nov(i,j) is shown in Tab. 5, 8, 11.

The set of Murphree efficiency coefficients (Tab.6, 9, 12) is obtained for each component by each tray corresponding to calculated mass transfer coefficients.

Tab. 4 Tray Column Tray 2, Base Component = 3 Isopropylbenzene, M Matrix: M(i,j)

	1	2	3	4	5	6	7
1	7.8045e+000	-3.3801e-012	2.3419e-012	4.4095e-012	5.6774e-012	-1.2894e-011	1.0355e-012
2	-2.6999e-001	1.5829e+000	1.7013e-002	3.1204e-002	4.0508e-002	-9.3451e-002	7.7699e-003
3	-6.0980e-002	-5.4735e-003	5.8338e-001	6.4858e-003	8.6523e-003	-2.1087e-002	1.8433e-003
4	-5.9358e-003	-5.1447e-004	3.3883e-004	2.3230e-001	7.9088e-004	-2.0281e-003	1.8958e-004
5	-2.4940e-010	-2.1418e-011	1.4323e-011	2.4442e-011	3.5550e-003	-8.6122e-011	7.8111e-012
6	-2.8635e-010	-2.6174e-011	1.8452e-011	3.3733e-011	4.3580e-011	3.3565e+000	8.1253e-012
7	-1.3178e-002	-1.1810e-003	8.5121e-004	1.5014e-003	1.9691e-003	-4.5537e-003	8.0178e-001

Tab. 5 Overall number of transfer units: Nov(i,j) Tray 2

	1	2	3	4	5	6	7
1	5.6496e-001	1.3032e-013	-3.8401e-014	-1.2421e-013	-8.1903e-014	4.4447e-013	-3.3397e-014
2	7.3898e-003	7.2735e-001	2.8675e-004	9.1138e-004	2.8457e-003	2.4972e-003	-3.2837e-004
3	1.1347e-003	-6.4170e-005	7.2101e-001	8.8753e-004	1.8162e-003	1.9437e-004	2.7706e-005
4	-3.5284e-005	-6.1968e-005	7.5360e-005	6.8402e-001	4.0679e-004	-8.8864e-005	1.4693e-006
5	-6.1737e-010	-2.3171e-010	2.1757e-010	6.3528e-010	6.3582e-001	-4.6415e-010	2.1090e-011
6	8.0937e-012	6.2942e-013	3.0671e-014	1.5401e-013	1.5107e-012	6.8122e-001	-3.4356e-013
7	2.9563e-004	-8.9860e-006	3.9095e-005	1.1566e-004	2.6636e-004	7.1276e-005	7.3477e-001

Tab. 6 Murphree Efficiencies Tray 2

	Component	Yin	Yout	Y*=(K*X)	Efficiency
1	Benzene	3.3248e-013	2.5347e-012	5.4327e-012	4.3179e-001
2	Ethylbenzene	2.9987e-002	3.4947e-002	3.9587e-002	5.1667e-001
3	Isopropylbenzene	9.5183e-001	9.5012e-001	9.4862e-001	5.3214e-001
4	Sec-Butylbenzene	1.3161e-002	1.1012e-002	8.9790e-003	5.1401e-001
5	M-DiisopropylBz	2.7753e-003	1.8353e-003	8.7884e-004	4.9565e-001
6	23-2C1-23-2PhnC4	6.8988e-009	3.6681e-009	3.6953e-011	4.7082e-001
7	Toluene	2.2758e-011	3.2242e-011	4.1951e-011	4.9415e-001
8	N-Propylbenzene	2.2439e-003	2.0839e-003	1.9369e-003	5.2113e-001

Tab. 7 Tray Column Tray 30, Base Component = 5 M-DiisopropylBz, M Matrix: M(i,j)

	1	2	3	4	5	6	7
1	1.7919e+001	-1.2775e-013	-7.5977e-014	-3.4231e-014	2.8513e-014	-2.5135e-013	-6.0674e-014
2	-1.0086e-004	5.1980e+000	-1.4979e-005	-6.7278e-006	5.5743e-006	-4.9393e-005	-1.1959e-005
3	-1.2373e-001	-3.0732e-002	3.4779e+000	-8.2119e-003	6.8828e-003	-6.0547e-002	-1.4607e-002
4	-1.5688e-001	-3.8967e-002	-2.3193e-002	2.1066e+000	8.7372e-003	-7.6737e-002	-1.8403e-002
5	-1.0002e-002	-2.4889e-003	-1.4917e-003	-6.7062e-004	3.9347e-002	-4.9044e-003	-1.1861e-003
6	-8.5511e-016	-2.1266e-016	-1.2688e-016	-5.6937e-017	4.7315e-017	9.2823e+000	-1.0101e-016
7	-1.2403e-003	-3.0866e-004	-1.8368e-004	-8.2869e-005	6.8866e-005	-6.0730e-004	2.9942e+000

Tab. 8 Overall number of transfer units: Nov(i,j) Tray 30

	1	2	3	4	5	6	7
1	4.9290e-001	4.1845e-015	2.7981e-015	1.7716e-015	-1.0271e-015	6.4935e-015	2.2914e-015
2	2.9359e-006	8.2840e-001	8.3570e-007	5.3015e-007	-2.5992e-007	2.0314e-006	6.6730e-007
3	3.8137e-003	1.6013e-003	8.9938e-001	6.5781e-004	-2.6555e-004	2.6015e-003	8.1135e-004
4	5.0609e-003	2.1309e-003	1.4366e-003	9.6659e-001	2.3412e-004	3.4259e-003	1.1373e-003
5	2.9240e-004	9.8148e-005	6.0380e-005	4.9399e-005	9.9482e-001	1.8077e-004	4.0386e-005
6	2.1208e-017	9.6280e-018	6.4004e-018	3.9980e-018	-2.6218e-018	6.8042e-001	5.2285e-018
7	3.9199e-005	1.6163e-005	1.0365e-005	6.5215e-006	-2.4801e-006	2.6544e-005	9.3181e-001

Tab. 9 Murphree Efficiencies Tray 30

	Component	Yin	Yout	Y* = (K*X)	Efficiency
1	Benzene	1.7190e-015	1.2850e-014	3.0298e-014	3.8948e-001
2	Ethylbenzene	1.5195e-006	4.0221e-006	5.9583e-006	5.6378e-001
3	Isopropylbenzene	2.7716e-003	5.4638e-003	7.3086e-003	5.9338e-001
4	Sec-Butylbenzene	5.8043e-003	7.9523e-003	9.2667e-003	6.2037e-001
5	M-DiisopropylBz	9.9079e-001	9.8593e-001	9.8275e-001	6.0506e-001
6	23-2C1-23-2PhnC4	5.9851e-004	5.9373e-004	5.9064e-004	6.0846e-001
7	Toluene	4.4083e-019	2.5171e-017	5.0505e-017	4.9398e-001

Tab. 10 Tray Column Tray 61, Base Component = 5 M-DiisopropylBz, M Matrix: M(i,j)

	1	2	3	4	5	6	7
1	1.6227e+001	-4.2917e-013	-2.5826e-013	-1.1650e-013	1.0248e-013	-8.2729e-013	-2.0790e-013
2	-2.5300e-013	4.9581e+000	-3.9680e-014	-1.7932e-014	1.5453e-014	-1.2704e-013	-3.2049e-014
3	-8.0878e-011	-2.1105e-011	3.3872e+000	-5.7401e-012	5.0067e-012	-4.0607e-011	-1.0204e-011
4	-6.5249e-006	-1.7019e-006	-1.0236e-006	2.0728e+000	4.0505e-007	-3.2736e-006	-8.2364e-007
5	-1.1372e-002	-2.9728e-003	-1.7897e-003	-8.1514e-004	4.5574e-002	-5.7224e-003	-1.4532e-003
6	-1.8972e-014	-4.9488e-015	-2.9800e-015	-1.3476e-015	1.1709e-015	8.6435e+000	-2.3939e-015
7	-2.3254e-011	-6.0617e-012	-3.6521e-012	-1.6483e-012	1.4307e-012	-1.1672e-011	2.9231e+000

Tab. 11 Overall number of transfer units: Nov(i,j) Tray 61

	1	2	3	4	5	6	7
1	5.3110e-001	1.5787e-014	1.0678e-014	7.0235e-015	-4.1512e-015	2.4235e-014	8.7408e-015
2	8.2663e-015	8.6226e-001	2.4200e-015	1.6128e-015	-8.0360e-016	5.7206e-015	1.9349e-015
3	2.7926e-012	1.1950e-012	9.3098e-001	5.2937e-013	-2.2233e-013	1.9087e-012	6.1916e-013
4	2.3859e-007	1.0526e-007	7.3365e-008	1.0005e+000	1.0551e-008	1.6338e-007	5.9143e-008
5	7.7905e-005	-1.6421e-004	-1.5328e-004	-9.8441e-005	1.0348e+000	-8.4385e-005	-1.8063e-004
6	5.2391e-016	2.3395e-016	1.5562e-016	9.9810e-017	-6.4329e-017	7.1686e-001	1.2534e-016
7	8.2268e-013	3.4674e-013	2.2668e-013	1.5121e-013	-6.2096e-014	5.5882e-013	9.6428e-001

Tab. 12 Murphree Efficiencies Tray 61

	Component	Yin	Yout	Y* = (K*X)	Efficiency
1	Benzene	6.5948e-015	4.8474e-014	1.0822e-013	4.1208e-001
2	Ethylbenzene	4.1544e-015	1.1355e-014	1.6616e-014	5.7784e-001
3	Isopropylbenzene	1.8942e-012	3.9659e-012	5.3135e-012	6.0589e-001
4	Sec-Butylbenzene	2.3728e-007	3.5823e-007	4.2858e-007	6.3227e-001
5	M-DiisopropylBz	9.9712e-001	9.9850e-001	9.9925e-001	6.4473e-001
6	23-2C1-23-2PhnC4	2.8762e-003	1.5034e-003	7.4692e-004	6.4470e-001
7	Toluene	1.8317e-016	7.2723e-016	1.2463e-015	5.1177e-001
8	N-Propylbenzene	6.2265e-013	1.1822e-012	1.5270e-012	6.1880e-001

The rigorous calculation of mass transfer by using SRK phase equilibrium model allows to determine actual columns pressure drop, heat duties, trays compositions and temperature profiles. The comparison of real industrial and simulated data for all columns is presented in the next section.

Flowsheet simulation applying tray efficiencies

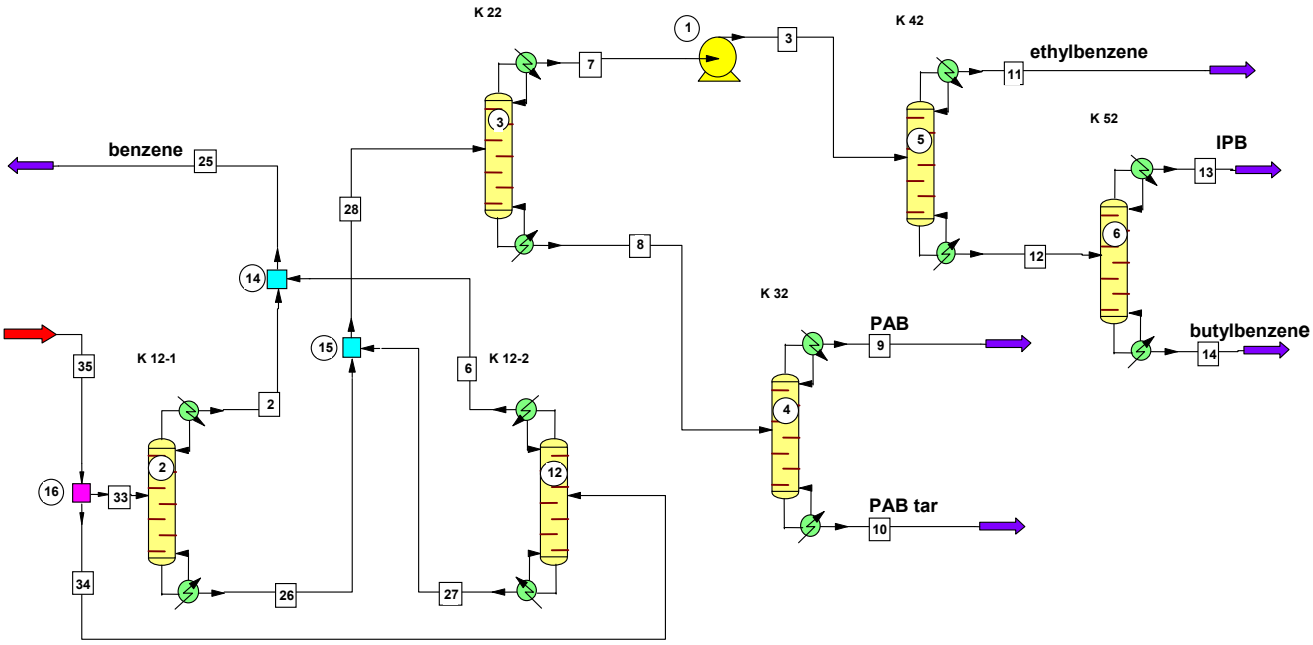


Fig.2 Calculated scheme [3]

Because of extremely durable computing of many different variants of complicated mixtures it is reasonable to use efficiencies instead of mass transfer mode. The linearization of obtained Murphree's efficiency coefficients was applied to components separation in a column from the top tray to the bottom tray.

As shown in Tab.6, 9, 12 Murphree's efficiency coefficients for each component are different and for linearization there were used key splitting components by columns. The comparative analysis of rigorous mass transfer and key component efficiencies modeling gives good correspondence (as shown below for column K 22) for the possibility of simulating the process (Tab. 13).

Tab. 13

	Actual feed tray mass transfer			Actual feed tray efficiency				
Tray # 1	109,54 C	0,29 atm		109,53 C	0,29 atm			
	Vap kmol/h	Liq kmol/h	Y/X	Vap kmol/h	Liq kmol/h	Y/X	deflection vapor(%)	deflection liquid(%)
Benzene	0	0,00004	0	0	0,00004	0		
Ethylbenzene	0	34,1316	0	0	35,33172	0		
Isopropylbenzene	0	914,6491	0	0	946,3243	0		
Sec-Butylbenzene	0	8,57345	0	0	8,80347	0		
M-DiisopropylBz	0	1,77367	0	0	1,83604	0		
23-2C1-23-2PhnC4	0	0,0002	0	0	0,00006	0		
Toluene	0	0,00006	0	0	0,00002	0		
N-Propylbenzene	0	2,00189	0	0	2,07056	0		
Total kmol/h	0	961,1301		0	994,3664		0,00%	-3,46%
Tray # 2	109,50 C	0,29 atm		109,54 C	0,29 atm			
	Vap kmol/h	Liq kmol/h	Y/X	Vap kmol/h	Liq kmol/h	Y/X		
Benzene	0,00004	0,0001	0,30498	0,00004	0,00004	0,93081		
Ethylbenzene	39,77644	35,61768	0,9564	40,97657	35,01965	1,00685		
Isopropylbenzene	1065,91809	911,6447	1,00133	1097,51587	944,564	0,99981		
Sec-Butylbenzene	9,99137	8,31964	1,02848	10,20998	8,82908	0,99506		
M-DiisopropylBz	2,06701	1,69095	1,04686	2,12937	1,84879	0,99107		
23-2C1-23-2PhnC4	0,00023	0,00019	1,05481	0,00008	0,00007	0,98846		
Toluene	0,00007	0,00007	0,81003	0,00003	0,00002	1,02694		
N-Propylbenzene	2,33297	1,96927	1,01457	2,40136	2,0713	0,9976		
Total kmol/h	1120,0862	959,2425		1153,2335	992,333		-2,96%	-3,45%
Tray # 61	174,30 C	0,50 atm		174,30 C	0,50 atm			
	Vap kmol/h	Liq kmol/h	Y/X	Vap kmol/h	Liq kmol/h	Y/X		
Benzene	0	0	0,83884	0	0	0		
Ethylbenzene	0,00285	0,00134	2,24419	0,00235	0,00101	2,46018		
Isopropylbenzene	5,88138	3,35321	1,85222	5,85978	3,2761	1,8849		
Sec-Butylbenzene	14,32268	10,5454	1,43429	14,8503	11,1716	1,40083		
M-DiisopropylBz	951,45673	1007,142	0,99764	981,6308	1037,038	0,99751		
23-2C1-23-2PhnC4	1,52814	6,71664	0,24026	1,86219	6,80267	0,28848		
Toluene	0	0	2,85896	0	0	0		
N-Propylbenzene	0,09229	0,0566	1,72183	0,09679	0,0595	1,71426		
Total kmol/h	973,284	1027,815		1004,3022	1058,349		-3,19%	-2,97%
Tray # 62	177,00 C	0,50 atm		177,00 C	0,50 atm			
	Vap kmol/h	Liq kmol/h	Y/X	Vap kmol/h	Liq kmol/h	Y/X		
Benzene	0	0	1,02762	0	0	0		
Ethylbenzene	0,00132	0,00002	5,07784	0,00099	0,00001	5,0765		
Isopropylbenzene	3,28536	0,06785	3,47789	3,21185	0,06426	3,47781		
Sec-Butylbenzene	10,20167	0,34373	2,13169	10,81848	0,35311	2,1317		
M-DiisopropylBz	942,73096	64,41068	1,05123	972,65973	64,37819	1,05123		
23-2C1-23-2PhnC4	2,66547	4,05118	0,04726	2,75148	4,0512	0,04726		
Toluene	0	0	8,82527	0	0	0		
N-Propylbenzene	0,05528	0,00132	3,00366	0,05815	0,00135	3,00365		
Total kmol/h	958,9401	68,8748		989,5007	68,8481		-3,19%	0,04%

The results obtained using mass transfer and key component efficiency linearization are shown in Tab. 14, 15 and the comparison of condenser and reboiler duties for both cases is shown in Tab. 16. It is clear that the difference of values is not significant.

Tab. 14 Calculated properties of columns Rigorous Distillation Summary using mass transfer

Equip. No.	2	12	3	4	5	6
Name	K 12-1	K 12-2	K 22	K 32	K 42	K 52
No. of trays (with condenser and reboiler)	58	58	62	30	62	62
1st feed tray	21	21	45	23	21	41
Colm press drop atm	0,21	0,21	0,2149	0,1632	0,2323	0,2904
Top pressure atm	1,2417	1,2417	0,2851	0,0382	1,1227	1,0453
Condenser duty kcal/h	-1 738 500	-1 738 700	-10 726 000	-931 171	-4 093 600	-17 511 000
Reblr duty kcal/h	2 533 200	2 533 500	10 042 000	514 820	4 617 600	17 412 000
Reflux mole kmol/h	19,7651	19,255	961,1301	18,9271	465,6307	1806,8733
Reflux ratio	0,093	0,0906	6,0465	0,3	71,4262	12
Reflux mass kg/h	1571,795	1531,1512	115238,211	3067,587	50405,188	217160,469
Column diameter m	2,6	2,6	3	1,6	3	3
Tray space m	0,4	0,4	0,4	0,6096	0,35	0,4

Tab.15 Distillation Summary using key component efficiency coefficients linearization

Equip. No.	2	12	3	4	5	6
Name	K 12-1	K 12-2	K 22	K 32	K 42	K 52
No. of trays	58	58	62	30	62	62
actual l feed tray	21	21	45	23	21	41
Colm press drop (kg/cm2)	0,217	0,217	0,222	0,1686	0,24	0,3
Efficiency top tray	0,58	0,58	0,01	0,25	0,52	0,462
Efficiency bot tray	0,67	0,67	0,37	0,45	0,6	0,372
Top pressure kg/cm2	1,283	1,283	0,2946	0,0394	1,16	1,08
Cond duty kcal/h	-1 737 400	-1 737 400	-10 936 000	-930 534	-4 089 500	-17 466 000
Reblr duty kcal/h	2 532 200	2 532 200	10 172 000	514 723	4 618 000	17 345 000
Reflux mole kmol/h	19,66	19,6597	982,8221	18,9278	465,4855	1801,6548
Reflux ratio	0,0925	0,0925	6,1833	0,3	73,4511	11,947
Reflux mass kg/h	1563,4019	1563,3838	117838,28	3067,63	50415,875	216507,7

Tab.16 Condenser and reboiler duties comparison by using Rigorous Distillation of mass-transfer and key component efficiency coefficients linearization (see Tab.14, 15)

Cond duty difference	**0,06%**	**0,07%**	**-1,96%**	**0,07%**	**0,10%**	**0,26%**
Reblr duty difference	**0,04%**	**0,05%**	**-1,29%**	**0,02%**	**-0,01%**	**0,38%**

The calculated results of material balance by using **key component** efficiency coefficients linearization for flowsheet simulation is shown in Tab. 17.

Tab.17 Calculated properties of main streams for actual flowsheet

Stream No.	35	25	28	3	12	13	14	8	9	10
Temp C	80	88,5412	177,877	109,5724	164,8562	154,2959	187,1302	177	97,3209	182,9813
Pres atm	1,9357	1,2417	1,4518	1,9357	1,355	1,0453	1,3356	0,5	0,0382	0,2013
Total kg/h	64325,12	33794,49	30530,66	19058,626	18352,9533	18096,8366	256,1107	11472,0394	10225,2947	1246,7435
Component mass %										
Benzene	49,71287	94,62454	0	0	0	0	0	0	0	0
Ethylbenzene	1,149316	0,414268	1,962943	3,144495	0,054486	0,055257	0,00001	0,000017	0,000019	0
Isopropylbenzene	30,66092	4,536004	59,57868	95,398331	98,432446	99,730289	6,726743	0,071085	0,079751	0,000007
Sec-Butylbenzene	0,378545	0,020861	0,774468	0,998574	1,036958	0,004353	74,00105	0,402157	0,451064	0,001046
M-DiisopropylBz	16,32424	0,003242	34,39001	0,249755	0,259358	0	18,585667	91,107577	99,463093	22,578953
23-2C1-23-2PhnC4	1,501278	0	3,163048	0,000042	0,000043	0	0,003093	8,417782	0,004523	77,419996
Toluene	0,207228	0,39444	0,000003	0,000005	0	0	0	0	0	0
N-Propylbenzene	0,065604	0,00665	0,130861	0,208797	0,216709	0,210104	0,683439	0,001385	0,001554	0

The results shown in Tab.17 correspond to the real data. It allows to solve the problem of improving parameters of the actual industrial flowsheet.

Feed trays optimization

Since for operating plants energy saving is highly important, the reboiler duty of column was chosen as objective function for optimization. The sensitivity analysis of model parameters of the columns was carried out. It was found out that the objective function mostly depends on feed tray position. The results of this analysis for all columns are present in the graphics (Fig 3 - 6). However, in order to choose the optimal feed trays it is also necessary to take into account the influence of other important factors such as losses of main component (IPB) and impurities. The final results of this investigation are shown in Tab.18.

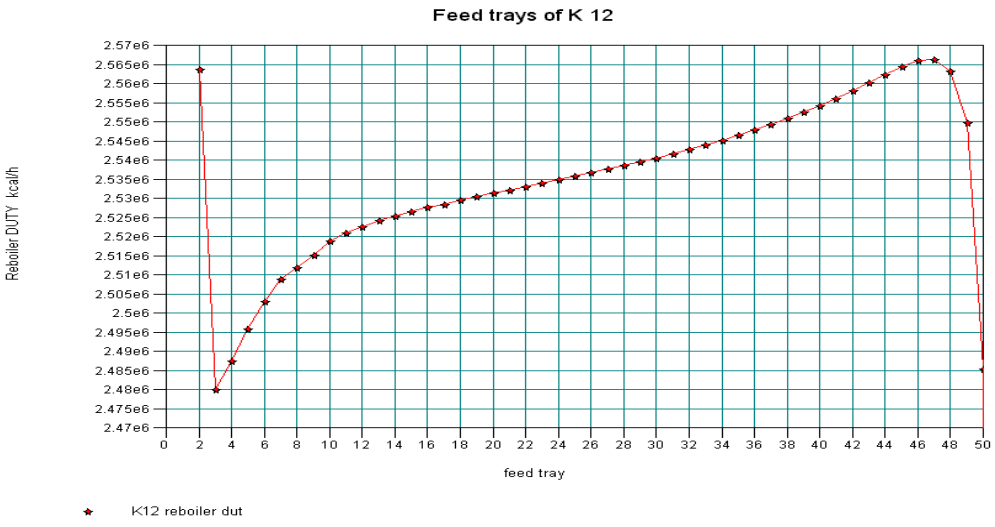


Fig. 3

For columns K 12(1, 2) the 15-th tray for feed stream was chosen due to significant increasing of IPB contents (up to 5,8% by wt.) in recycle stream of benzene at higher feed trays. (Fig. 3)

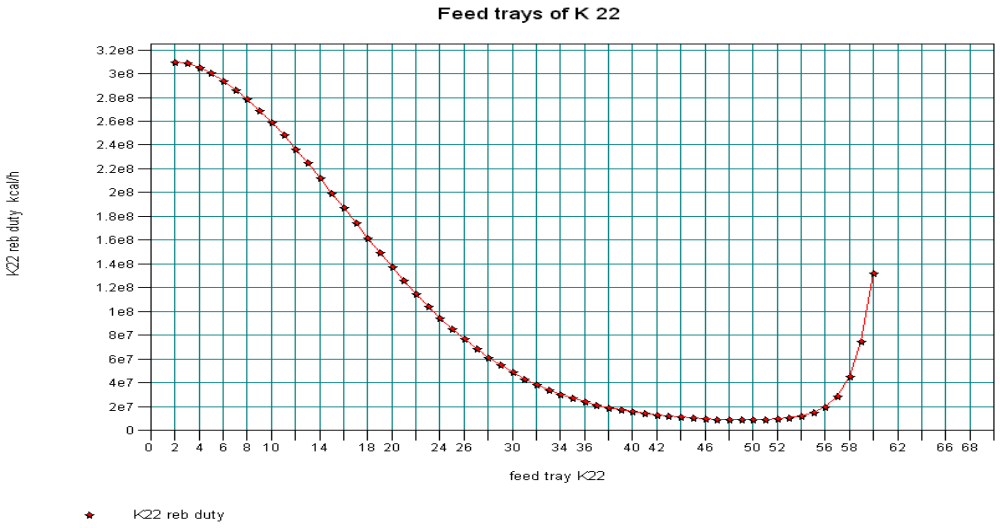


Fig.4

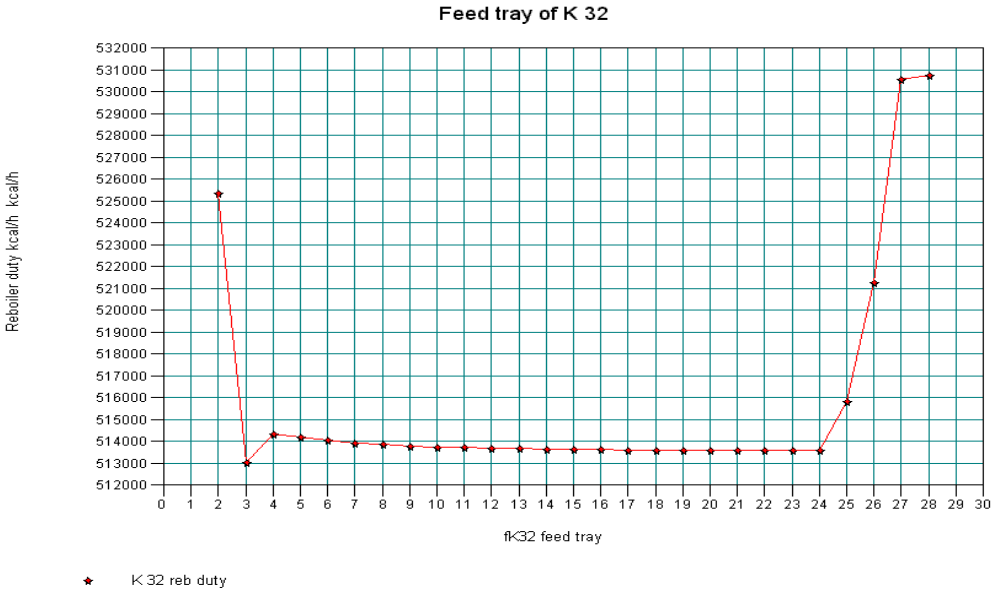


Fig.5

As shown in Fig.5 there is no significant reboiler duty dependence on feed tray number in the range from 3 up to 24 trays. There is minimum heat consumption at two optimal feed trays 3 or 24, but the 24-th was chosen because the 3-rd tray increased the amount of heavy PAB tar in the PAB distillate. The points corresponding to 27-28 trays are the result of divergence.

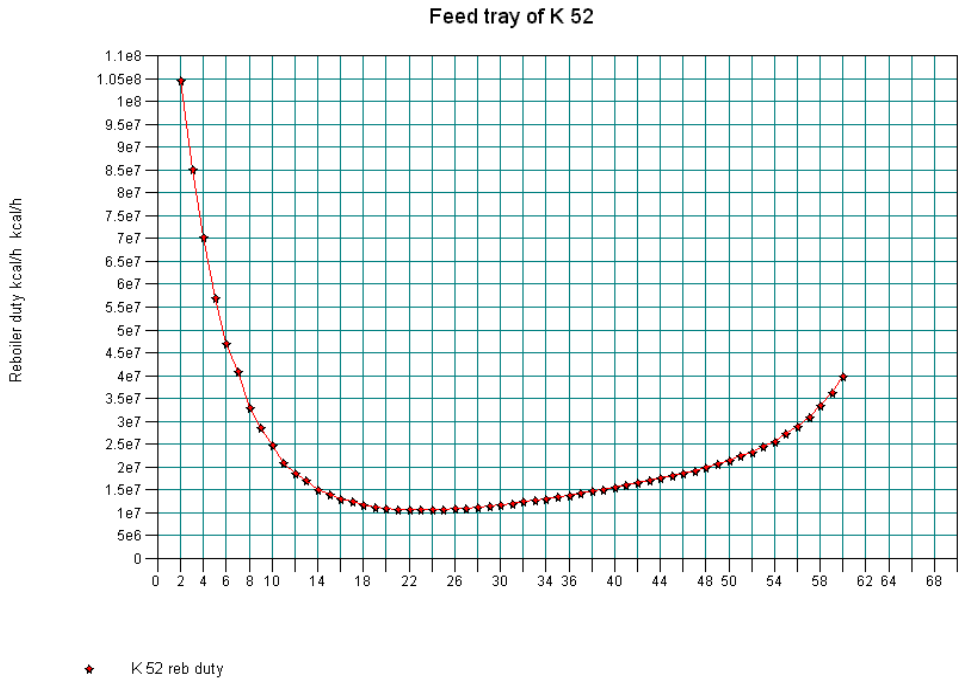


Fig.6

Tab.18 Optimal feed trays Distillation Summary

Equip. No.	2	12	3	4	5	6
Name	K 12-1	K 12-2	K 22	K 32	K 42	K 52
No. of trays	58	58	62	30	62	62
optimal feed tray	15	15	50	24	29	25
Efficiency top tray	0,58	0,58	0,01	0,25	0,52	0,462
Efficiency bot tray	0,67	0,67	0,37	0,45	0,6	0,372
Cond duty kcal/h	-1 731 700	-1 732 200	-9 692 900	-929 773	-3 633 900	-10 784 000
Reblr duty kcal/h	2 526 300	2 525 800	8 924 800	513 599	4 164 200	10 685 000
Reflux mole kmol/h	18,7344	18,8124	853,079	18,9107	412,9195	1054,7747
Reflux ratio	0,0881	0,0885	5,3688	0,3	65,1609	7
Reflux mass kg/h	1490,0635	1496,293	102285,7344	3064,99	44722,5625	126754,1641

The comparative result of heat consumption (condenser and reboiler duties) by feed tray changing from actual to optimal is shown in Tab.19, 20.

Tab.19 Actual feed trays Distillation Summary (see Tab.14)

Cond duty kcal/h	-1 737 400	-1 737 400	-10 936 000	-930 534	-4 089 500	-17 466 000
Reblr duty kcal/h	2 532 200	2 532 200	10 172 000	514 723	4 618 000	17 345 000
Cond duty difference kcal/h	5 700,00	5 200,00	1 243 100,00	761,00	455 600,00	6 682 000,00
Reblr duty difference kcal/h	5 900,00	6 400,00	1 247 200,00	1 124,00	453 800,00	6 660 000,00

Tab. 20 Heat savings by feed trays positions changing from actual to optimal

Cond duty saving summary kcal/h	**8 392 361,00**	**22,7%**
Reblr duty saving summary kcal/h	**8 374 424,00**	**22,2%**

FLOWSHEET SYNTHESIS WITH ADDING WATER

Phase equilibrium modification

Because of high boiling temperature and possibility of polymerization and decomposition processes of some heavy hydrocarbons (Sec-Butylbenzene, M-DiisopropylBz, Polyalkylbenzene tar) during rectification, several columns are operated under vacuum. This requires extra energy for vacuum machines. Creation of artificial heteroazeotropic system by adding polar component could solve the high boiling temperature problem. The cheapest one is water, but its amount must be properly determined to obtain alternative water heating expenses which should be lower than vacuum process cost. As the thermodynamic model the UNIFAQ LLV equation was chosen because of insufficiency of BIPs data for NRTL or UNIQUAC. For indirect estimation of UNIFAQ LLV calculation there were used the known data for azeotropic systems.

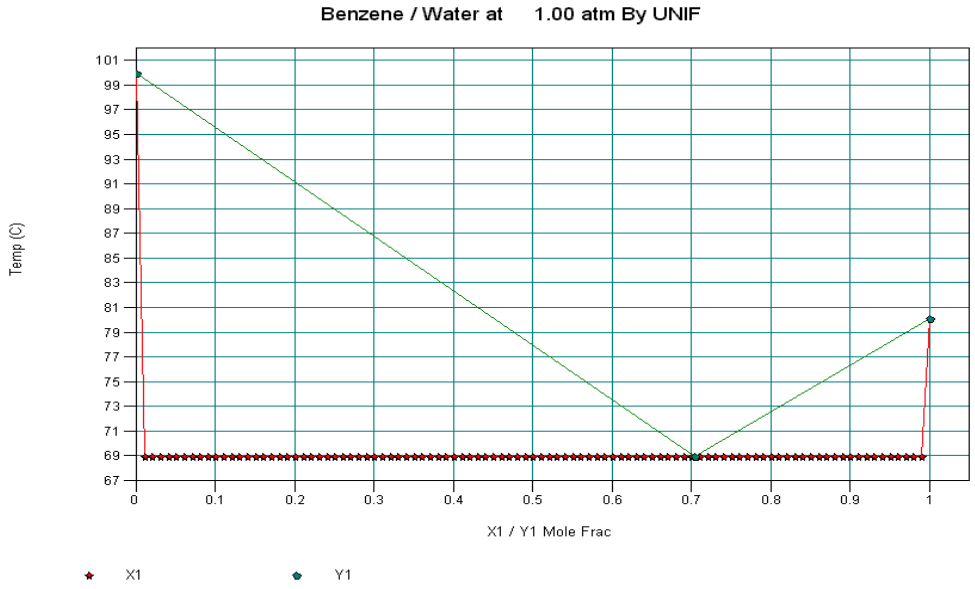


Fig.7

Calculated result: contents of benzene 70.0% mole, boiling temperature 68.99 C degree at the pressure of 1 atm. (Fig.7).
Actual result: contents of benzene 70.2% mole, boiling temperature 69.2 C degree at the pressure of 1 atm. [2]

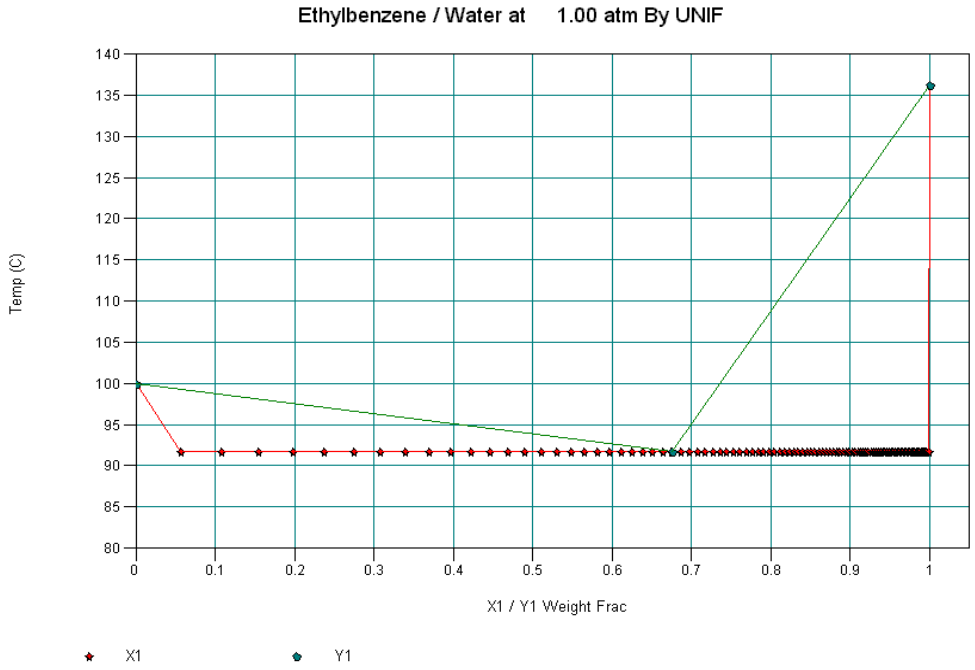


Fig.8

Calculated result: contents of ethylbenzene 68.0% mass, boiling temperature 91.69 C degree at the pressure of 1 atm. (Fig.8).
Actual result: contents of ethylbenzene 67.0% mass, boiling temperature 92.0 C degrees at the pressure of 1 atm. [2]

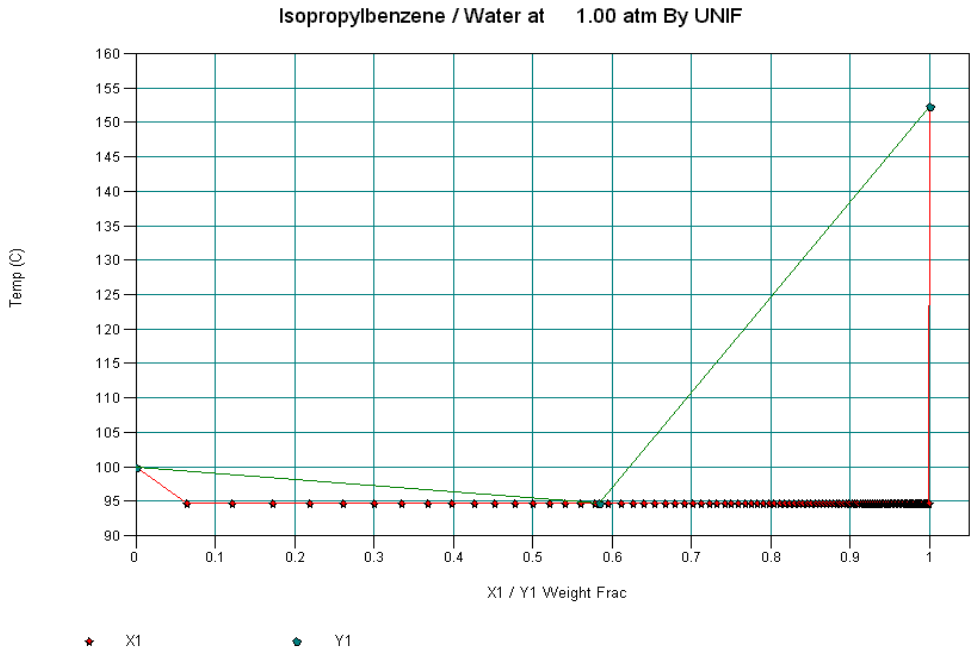


Fig.9

Calculated result: contents of isopropylbenzene 58.0% mass, boiling temperature 94.71 C degree at the pressure of 1 atm. (Fig. 9)
Actual result: contents of isopropylbenzene 56.2% mass, boiling temperature 95.0 C degrees at the pressure of 1 atm. [2]

To attain UNIFAQ LLV application for heteroazeotropic system extremely low solubility of these components at normal conditions was taken into account. That fact is shown (Fig. 10) at calculated binodal plot of water/isopropylbenzene/sec-butylbenzene system.

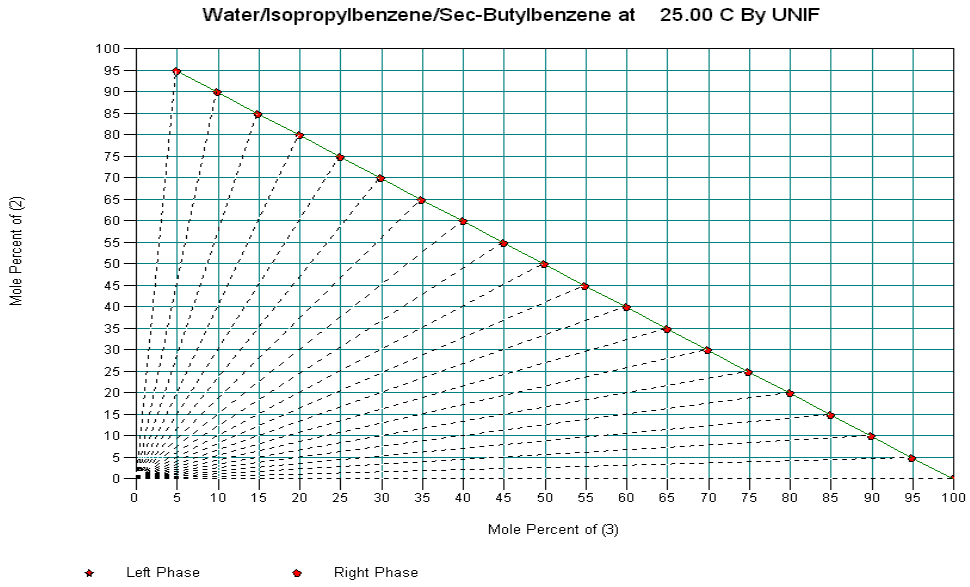


Fig.10

The obtained comparison makes it possible to use UNIFAC LLV for the following subordinated studies of water system for the described hydrocarbons.

Flowsheet modification
There are two vacuum columns in actual flowsheet K 22 and K 32 (Fig.2, section 3.3). One can get the most significant value of pressure change in column named K 32 (Tab. 14) since it is operated under deepest vacuum in the flowsheet as a result of heavy components distillation. But in our case it was not carried out because of unsolved problem of possible water presents in recycle PAB stream, anyway PAB fraction contains up to 300 ppm of water as a result of adding water into column K 52.

Water supply to column K 22 causes changes of flowsheet with different ways of obtaining final products. For example instead of simultaneous separation of IPB and Sec-butylbenzene at the column K 52 the variant of separation ethylbenzene and IPB was created with the corresponding modification of the whole flowsheet. For splitting water and organic phases after distillation columns the three decanters: units 11, 15 and 16 were added (Fig. 11).

The flowsheet with water added is presented:

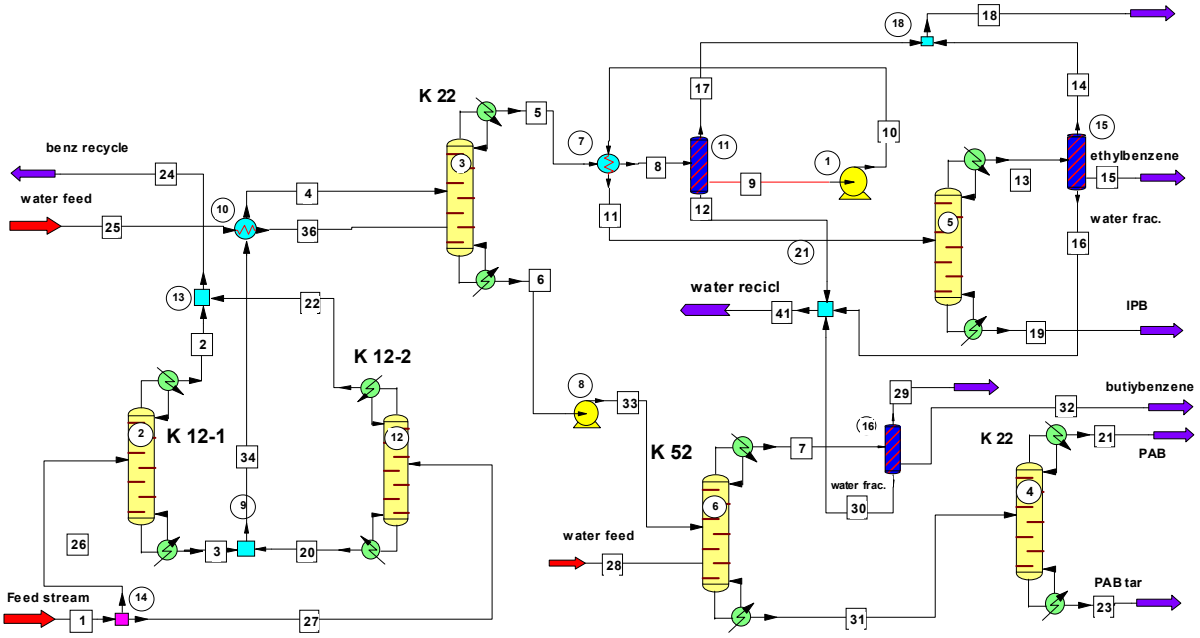


Fig. 11

For water use as an agent forming heteroazeotropic system the problem of water optimal amount must be solved. We have the situation than the number of components forms a complicated mixture with heteroazeotropic properties affecting obliquely energy consumption. To reveal the dependence of the major parameters of a column (reboiler duty, reflux mass, bottom product presence in distillate and other) on water feed the sensitivity study was carried out. The main aim of this calculation is to find the balance of increasing energy consumption because of distillate mass growths and decreasing of supplied heat due to boiling temperature coming down.

The simulation results with water adding to columns trays results in undesirable increasing of bottom temperature (see section 4.1) at the columns K 22 and K 52. Therefore the problem for definition of water feed stream parameters and entrance position to column has to be solved.

It was discovered that water and the main feed stream should be charged into the column separately. The sensitivity analyses of K 22 showed what reboiler duty (5,582–e6 kcal/h) does not depend on water feed tray number. The same is true with ethylbenzene level in the bottom stream (4, 79 kg/h) from 3 to 40 tray, the same case with IPB presents (4 395 kg/h).

The best way to add the water stream is to place it on the bottom of column. For the experiment calculated the column K 22 of polyalkylbenzenes distillation was used. To define the reboiler and condenser duties and bottom temperature in dependence on water amount added was carried out. The results, shown in Fig. 12 indicate linearly dependence of the reboiler and condenser duties on water feed amount.

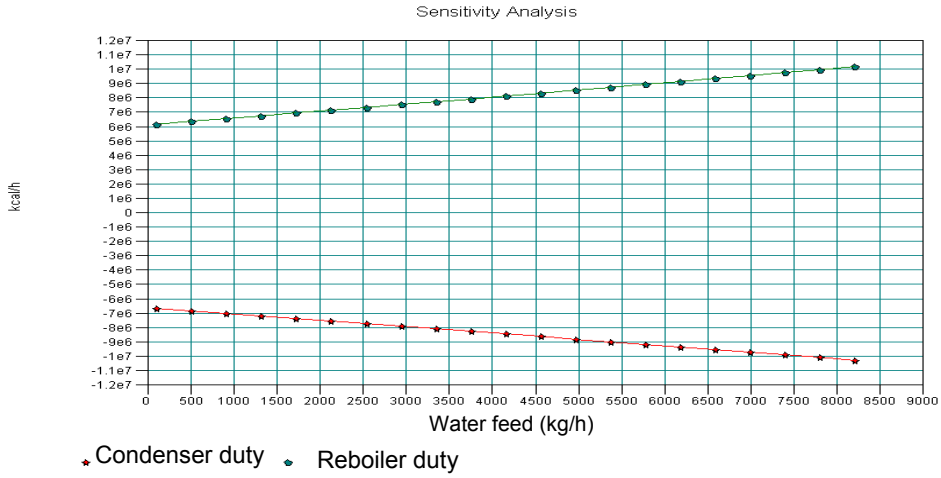


Fig. 12

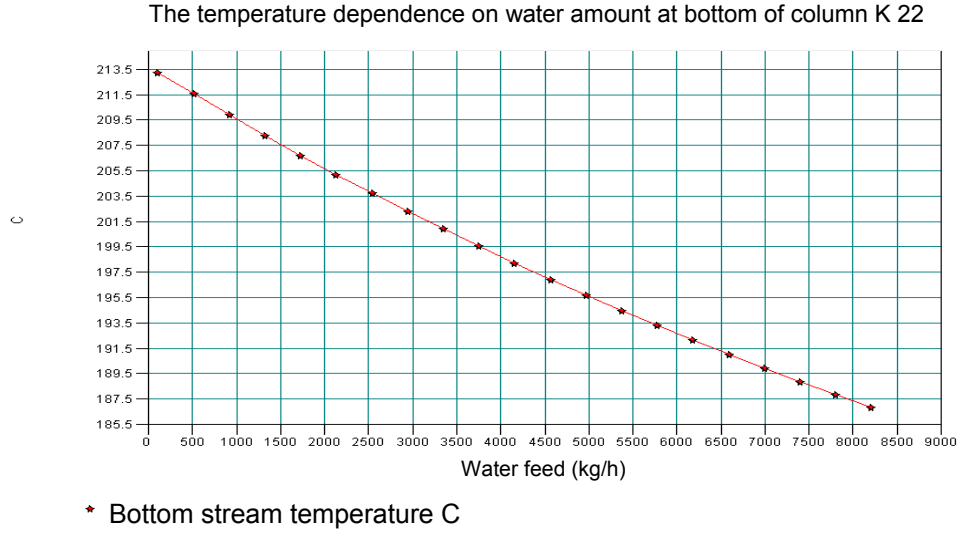


Fig.13

The heat dependence plot (Fig. 12) was used with temperature dependence on water amount (Fig. 13) to determine water flow to the column. It was found that for significant reducing the bottom temperature the flow of 1600 kg/h is enough. This allowed not to use vacuum equipment.

With adding water stream to the bottom of columns the azeotropic mixture is formed with boiling temperature minimizing and decreasing the bottom temperature more by 10-12 C.

The corresponding temperature profile of column K 22 and vapor composition profiles for columns K 52 and K 22 are presented in Fig. 14 , Fig. 15, Fig. 16.

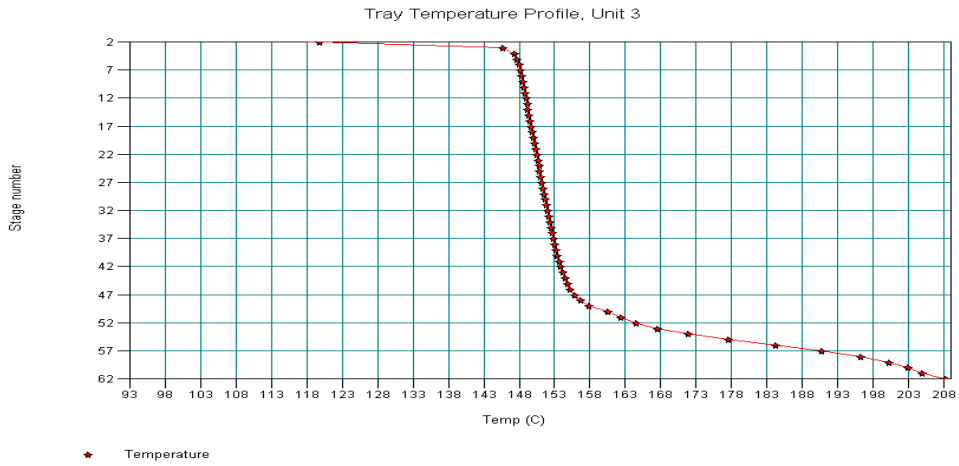


Fig. 14

The column vapor profile of K 22 and K 52 with water added is shown below.

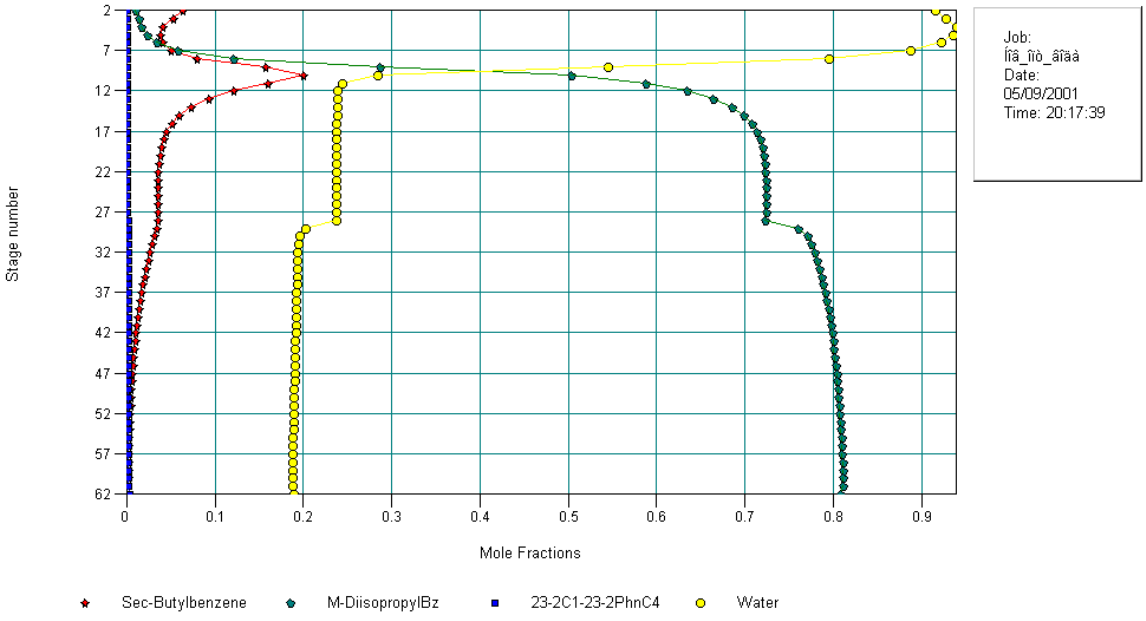


Fig. 15 Tray vapor profile of K 52

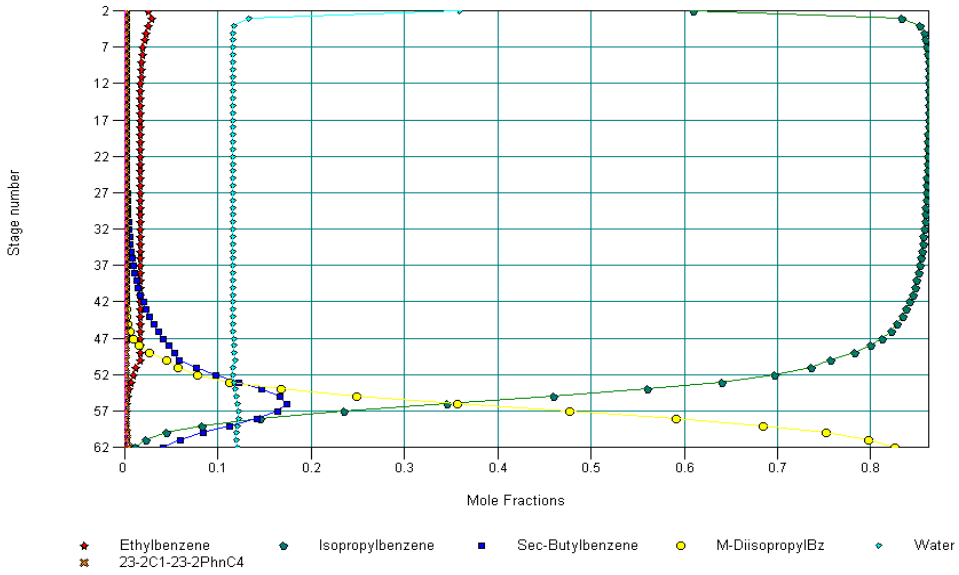


Fig.16 Tray vapor profile of K 22

HEAT RECUPERATION BY APPLYING ELEMENTS OF PINCH ANALYSIS

As seen from Fig.2 the flowsheet contains steams which obviously could be used as heating agents. The several types of possible flowsheets was been examined with water feed entering different points with using optimal heat consumption, and finally the variant using of pinch analysis [4-5] has been chosen (Fig. 17).

For heating reboiler of the vacuum column K 32 the bottom streams of the columns K 22 and K 12(1,2) were used. At the same time stream 23 was used for heating water feed. The column K 22 is operated under top pressure of 1 atm. without vacuum used previously.

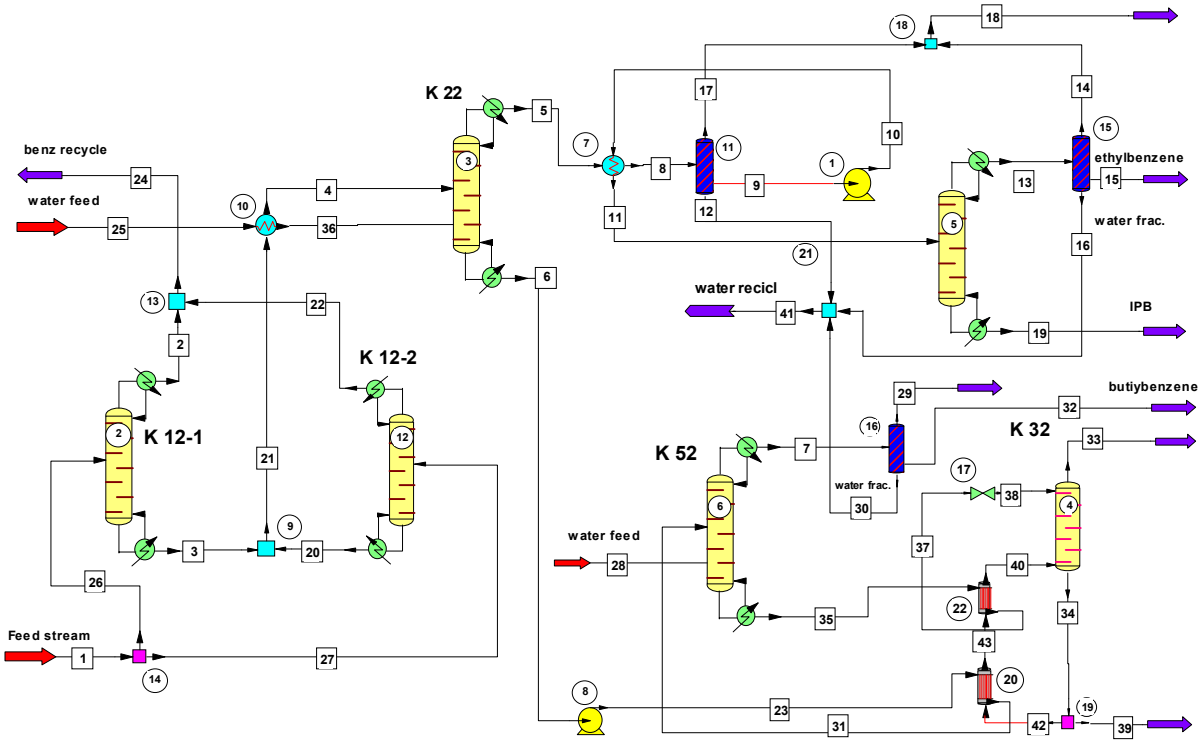


Fig. 17

Calculated results for all columns of final flowsheet are presented in Tab. 21, 22.

Tab. 21 Calculated results of product streams

	ethylbenzene fraction	IPB	butıybenzene fraction	PAB	PAB tar
Tempreture C	50	161,011	50	22,55 19	183,7676
Pressure atm.	1	1,242282	1	0,0381579	0,2013158
Vapor fraction	0	0	0	0	0
Enthalpy kcal/h	-1277,009	-308114,3	-33893,71	-1945584	17563,02
Total flow	759,2173	18140,71	311,9874	10279,02	1058,295
Total flow unit	kg/h	kg/h	kg/h	kg/h	kg/h
Component unit	weight fraction	weight fraction	weight fraction	weight fraction	weight fraction
Benzene	6,58379%	0,00000%	0,00000%	0,00000%	0,00000%
Ethylbenzene	81,00474%	0,08169%	0,00737%	0,00000%	0,00000%
Isopropylbenzene	1,03380%	99,69995%	11,98564%	0,00000%	0,00000%
Sec-Butylbenzene	0,00000%	0,00441%	74,24506%	0,02402%	0,00290%
M-DiisopropylBz	0,00000%	0,00000%	13,46201%	98,49480%	22,93692%
23-2C1-23-2PhnC4	0,00000%	0,00000%	0,00000%	1,45539%	77,06017%
Toluene	11,31638%	0,00000%	0,00000%	0,00000%	0,00000%
N-Propylbenzene	0,00011%	0,21395%	0,26040%	0,00000%	0,00000%
Water	0,06118%	0,00000%	0,03952%	0,02578%	0,00001%

Tab. 22 Distillation Summary for flowsheet with heat recuperation (kcal/h)

Name	K 12-1	K 12-2	K 22	K 42	K 52	K 32	units 11+15+16	Total
1st feed tray	3	3	50	26	28	30		
2nd feed tray	0	0	62	0	62	0		
Top pressure atm	1,2	1,2	1	1,01	1	0,0382		
Cond duty kcal/h	-1,73E+06	-1,73E+06	-7,60E+06	-5,67E+06	-1,08E+06	-1,58E+06	-155896,3	-1,95E+07
Reblr duty kcal/h	2,50E+06	2,50E+06	7,47E+06	6,31E+06	1,34E+06	1		2,01E+07
Absolute total sum of condenser and reboiler duties						**3,97E+07 kcal/h**		

The total heat duty is 3,97E+07 kcal/h and energy saving in comparison with the results of calculation for flowsheet without heat recuperation (4,02E+07 kcal/h) is not significant. All described variants of distillation flowsheets heat duties are presented in Fig. 18.

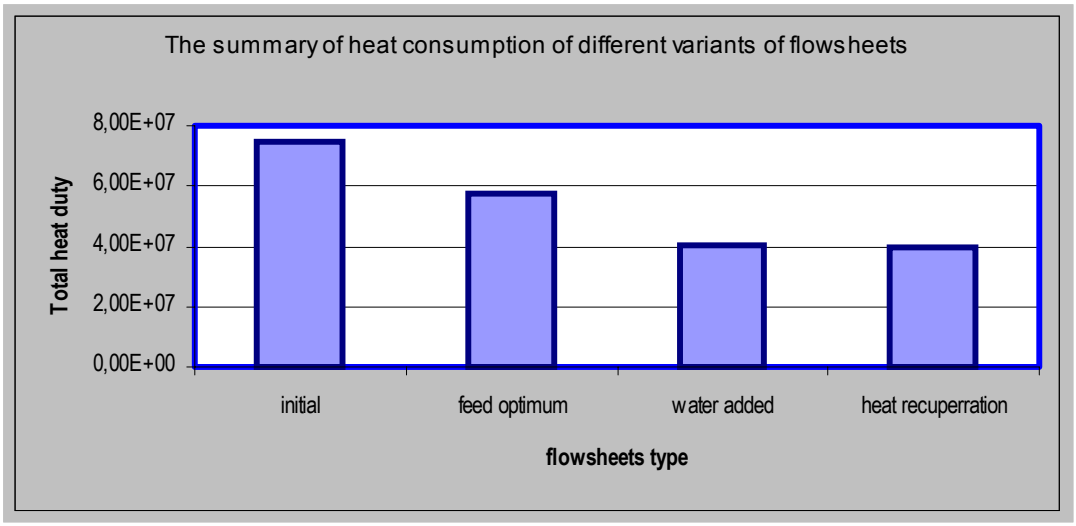


Fig.18

The final results of calculations lead to conclude that most reliable type of the flowsheet is the variant with adding water. The relative value of energy saving (reduction of total heat duty) in comparison with initial flowsheet is 46,2%.

CONCLUSION

The detailed investigation of isopropylbenzene distillation flowsheet syntheses in phenol-acetone production allows determining flowsheet energy savings. The sum of total heat consumption as an evidence of economical parameters gives the ground to consider the efficiency of technical solution involved. The use of combined method for flowsheet synthesis (feed tray optimization, adding water to the flowsheet and heat recuperation) makes it possible to obtain more efficient energy consumption close to 40-50% (relative) compared to original flowsheet data.

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