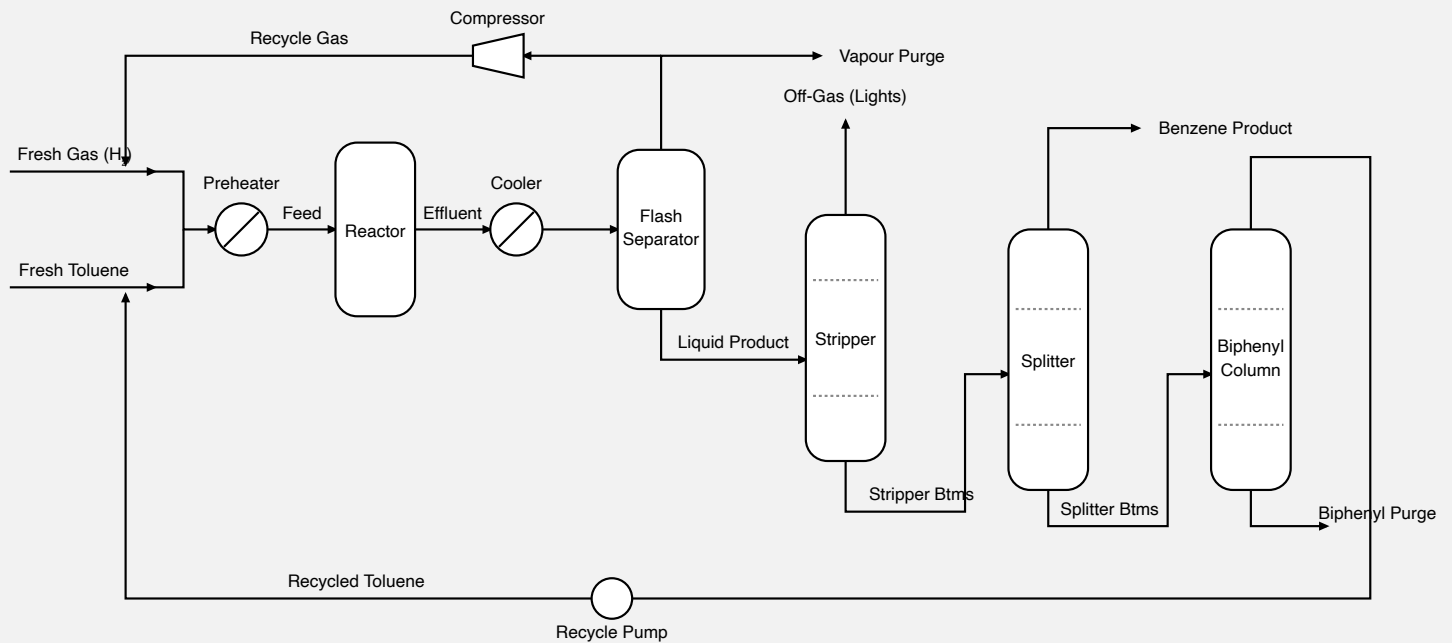


This example represents a process for producing benzene from toluene by means of hydrodealkylation, including the biphenyl side reaction. It demonstrates a conversion reactor with 2 reactions and a modification of the recycle model to handle two recycles.



Fresh gas feed at 35 °C, 35 bar (95% H₂, 5% CH₄)

freshGas

Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	35.00	35.00	35.00
p	kPa	3800.00	3800.00	3800.00
f	kmol/h	333.00	333.00	0.00
h	kJ/kmol	269.63	269.63	269.63
s	kJ/kmol-K	-27.67	-27.67	-27.67
hflow	W	24940.46412	24940.46412	0.00000
x	Hydrogen	0.95000	0.95000	0.95000
x	Methane	0.05000	0.05000	0.05000
x	Benzene	0.00000	0.00000	0.00000
x	Toluene	0.00000	0.00000	0.00000
x	Biphenyl	0.00000	0.00000	0.00000
massf	kg/h	904.83060	904.83060	0.00000
hflow	W	24940.46412	24940.46412	0.00000

Fresh liquid toluene feed.

freshTol

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	35.00	35.00	35.00
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	167.00	0.00	167.00
h	kJ/kmol	-35441.91	-35441.91	-35441.91
s	kJ/kmol-K	-93.28	-93.28	-93.28
hflow	W	-1644111.05280	0.00000	-1644111.05280
x	Hydrogen	0.00000	0.00000	0.00000
x	Methane	0.00000	0.00000	0.00000
x	Benzene	0.00000	0.00000	0.00000
x	Toluene	1.00000	1.00000	1.00000
x	Biphenyl	0.00000	0.00000	0.00000
massf	kg/h	15387.11781	0.00000	15387.11781
hflow	W	-1644111.05280	0.00000	-1644111.05280

Combines the gas and toluene streams along with the recycled gas and toluene.

MixedFeed

Label	Unit	B	V	L
q	Fraction	0.93392	1.00000	0.00000
t	degC	43.05	43.05	43.05
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	3494.99	3264.04	230.95
h	kJ/kmol	-1762.83	377.91	-32018.60
s	kJ/kmol-K	-26.06	-22.05	-82.73
hflow	W	-1711410.5	342640.9	-2054051.5
x	Hydrogen	0.48114	0.51376	0.02020
x	Methane	0.45156	0.48100	0.03539
x	Benzene	6.425799e-3	1.079116e-3	0.08199
x	Toluene	0.06087	4.164347e-3	0.86228
x	Biphenyl	9.819610e-6	3.425353e-9	1.485549e-4

massf	kg/h	50068.14935	30094.81512	19973.33424
hflow	W	-1711410.5	342640.9	-2054051.5

The reactor feed heated to 625 °C

ReactorFeed

Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	620.00	620.00	620.00
p	kPa	3400.00	3400.00	3400.00
f	kmol/h	3494.99	3494.99	0.00
h	kJ/kmol	29790.92	29790.92	29790.92
s	kJ/kmol-K	30.79	30.79	30.79
hflow	W	28921928.98491	28921928.98491	0.00000
x	Hydrogen	0.48114	0.48114	0.48114
x	Methane	0.45156	0.45156	0.45156
x	Benzene	6.425799e-3	6.425799e-3	6.425799e-3
x	Toluene	0.06087	0.06087	0.06087
x	Biphenyl	9.819610e-6	9.819610e-6	9.819610e-6
massf	kg/h	50068.14935	50068.14935	0.00000
hflow	W	28921928.98491	28921928.98491	0.00000

Thermal duty required to heat the mixed feed stream up to the reactor inlet temperature.

PreheaterQ 30633.33951 kW

An estimate of the gas recycle.

RecycleEst

Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	45.00	45.00	45.00
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	1500.00	1500.00	0.00
h	kJ/kmol	453.43	453.43	453.43
s	kJ/kmol-K	-21.71	-21.71	-21.71
hflow	W	188928.5	188928.5	0.0

x	Hydrogen	0.54450	0.54450	0.01234
x	Methane	0.44550	0.44550	0.04503
x	Benzene	9.900000e-3	9.900000e-3	0.86882
x	Toluene	9.900000e-5	9.900000e-5	0.02266
x	Biphenyl	9.900000e-7	9.900000e-7	0.05115
massf	kg/h	13540.71640	13540.71640	0.00000
hflow	W	188928.5	188928.5	0.0

An estimate of the toluene recycle stream.

RecycleTolEst				
Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	100.00	100.00	100.00
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	40.00	40.00	0.00
h	kJ/kmol	-25009.23	-25009.23	-25009.23
s	kJ/kmol-K	-61.96	-61.96	-61.96
hflow	W	-277880.30579	-277880.30579	0.00000
x	Hydrogen	9.970090e-11	9.970090e-11	9.970090e-11
x	Methane	9.970090e-11	9.970090e-11	9.970090e-11
x	Benzene	9.970090e-3	9.970090e-3	9.970090e-3
x	Toluene	0.98704	0.98704	0.98704
x	Biphenyl	2.991027e-3	2.991027e-3	2.991027e-3
massf	kg/h	3687.36939	3687.36939	0.00000
hflow	W	-277880.30579	-277880.30579	0.00000

Recycled liquid toluene.

RecycledToluene				
Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	109.05	109.05	109.05
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	44.02	0.00	44.02
h	kJ/kmol	-23385.09	-23385.09	-23385.09

s	kJ/kmol-K	-57.83	-57.83	-57.83
hflow	W	-285963.98500	0.00000	-285963.98500
x	Hydrogen	8.174756e-22	8.174756e-22	8.174756e-22
x	Methane	8.169513e-22	8.169513e-22	8.169513e-22
x	Benzene	0.01076	0.01076	0.01076
x	Toluene	0.98847	0.98847	0.98847
x	Biphenyl	7.657060e-4	7.657060e-4	7.657060e-4
massf	kg/h	4051.60956	0.00000	4051.60956
hflow	W	-285963.98500	0.00000	-285963.98500

Reactor effluent cooled to condense aromatics.

CoolerOutlet

Label	Unit	B	V	L
q	Fraction	0.93816	1.00000	0.00000
t	degC	35.00	35.00	35.00
p	kPa	3300.00	3300.00	3300.00
f	kmol/h	3494.99	3278.85	216.14
h	kJ/kmol	-1830.21	87.44	-30921.48
s	kJ/kmol-K	-26.05	-22.37	-81.89
hflow	W	-1776824.7	79643.5	-1856468.3
x	Hydrogen	0.43462	0.46264	9.534706e-3
x	Methane	0.49903	0.52916	0.04200
x	Benzene	0.05199	7.449836e-3	0.72775
x	Toluene	0.01339	7.514106e-4	0.20514
x	Biphenyl	9.638971e-4	2.070978e-7	0.01558
massf	kg/h	50068.14769	33027.32376	17040.82393
hflow	W	-1776824.7	79643.5	-1856468.3

High-pressure flash vapour stream rich in hydrogen and methane available for recycle. Ir is 1 - the vapour purge fraction of the flashed vapour.

RecycleGas

Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	35.00	35.00	35.00

p	kPa	3300.00	3300.00	3300.00
f	kmol/h	2950.97	2950.97	0.00
h	kJ/kmol	87.44	87.44	-30921.48
s	kJ/kmol-K	-22.37	-22.37	-81.89
hflow	W	71679.2	71679.2	0.0
x	Hydrogen	0.46264	0.46264	9.534707e-3
x	Methane	0.52916	0.52916	0.04200
x	Benzene	7.449836e-3	7.449836e-3	0.72775
x	Toluene	7.514106e-4	7.514106e-4	0.20514
x	Biphenyl	2.070978e-7	2.070978e-7	0.01558
massf	kg/h	29724.59139	29724.59139	0.00000
hflow	W	71679.2	71679.2	0.0

Recycled gas stream compressed back to reactor loop pressure to be mixed with fresh feed.

HPRecycle				
Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	39.70	39.70	39.70
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	2950.97	2950.97	0.00
h	kJ/kmol	236.33	236.33	236.33
s	kJ/kmol-K	-22.37	-22.37	-22.37
hflow	W	193723.7	193723.7	0.0
x	Hydrogen	0.46264	0.46264	0.46264
x	Methane	0.52916	0.52916	0.52916
x	Benzene	7.449836e-3	7.449836e-3	7.449836e-3
x	Toluene	7.514106e-4	7.514106e-4	7.514106e-4
x	Biphenyl	2.070978e-7	2.070978e-7	2.070978e-7
massf	kg/h	29724.59139	29724.59139	0.00000
hflow	W	193723.7	193723.7	0.0

Fraction of separator vapour to purge

VPurgeFrac	0.1
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Fraction of aromatic hydrocarbons (benzene and toluene) retained in the process rather than lost to the

vapor purge.

BzAndTolRecovery	98.9 %
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Toluene overhead stream from biphenyl removal column \ pumped to reaction pressure (35 bar) for recycle back to the reactor feed.

CalcRecycleTo1

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	109.05	109.05	109.05
p	kPa	3500.00	3500.00	3500.00
f	kmol/h	44.02	0.00	44.02
h	kJ/kmol	-23385.09	-23385.09	-23385.09
s	kJ/kmol-K	-57.83	-57.83	-57.83
hflow	W	-285964.0	0.0	-285964.0
x	Hydrogen	8.174560e-22	8.174560e-22	8.174560e-22
x	Methane	8.169463e-22	8.169463e-22	8.169463e-22
x	Benzene	0.01076	0.01076	0.01076
x	Toluene	0.98847	0.98847	0.98847
x	Biphenyl	7.657060e-4	7.657060e-4	7.657060e-4
massf	kg/h	4051.60956	0.00000	4051.60956
hflow	W	-285964.0	0.0	-285964.0

Liquid stream from the flash separator containing crude benzene and unreacted toluene sent to the stabilizer column.

StripperFeed

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	35.00	35.00	35.00
p	kPa	3300.00	3300.00	3300.00
f	kmol/h	216.14	0.00	216.14
h	kJ/kmol	-30921.48	87.44	-30921.48
s	kJ/kmol-K	-81.89	-22.37	-81.89
hflow	W	-1856468.3	0.0	-1856468.3

x	Hydrogen	9.534706e-3	0.46264	9.534706e-3
x	Methane	0.04200	0.52916	0.04200
x	Benzene	0.72775	7.449838e-3	0.72775
x	Toluene	0.20514	7.514108e-4	0.20514
x	Biphenyl	0.01558	2.070978e-7	0.01558
massf	kg/h	17040.82393	0.00000	17040.82393
hflow	W	-1856468.3	0.0	-1856468.3

Distillation column to strip dissolved light gases (hydrogen and methane) overhead from liquid aromatics.

Stripper							
Stage	T degC	P kPa	V kmol/h	L kmol/h	Q W	Feeds kmol/h	Draws kmol/h
1	-0.85113	400.00000		11.25222	-144594.45795		V 11.25222
2	104.75239	402.22222	22.50444	15.67675	0.00000		
3	113.97283	404.44444	26.92897	295.55918	0.00000	216.13730	
4	137.81109	406.66667	90.67410	335.45824	0.00000		
5	138.59110	408.88889	130.57316	336.87529	0.00000		
6	138.85410	411.11111	131.99021	337.27491	0.00000		
7	139.11635	413.33333	132.38983	337.62530	0.00000		
8	139.42823	415.55556	132.74023	337.87089	0.00000		
9	139.95027	417.77778	132.98581	337.51782	0.00000		
10	141.62078	420.00000	132.63274		1044195.75926		L 204.88508

Stabilized liquid bottoms from the stripper column, free of light gases, fed to the benzene splitter.

StripperOvhds				
Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	-0.85	-0.85	-0.85
p	kPa	400.00	400.00	400.00
f	kmol/h	11.25	11.25	0.00
h	kJ/kmol	-956.86	-956.86	-35407.01
s	kJ/kmol-K	-10.29	-10.29	-100.94
hflow	W	-2990.8	-2990.8	0.0
x	Hydrogen	0.18315	0.18315	3.122686e-4
x	Methane	0.80674	0.80674	0.01043

x	Benzene	0.01000	0.01000	0.94696
x	Toluene	1.132458e-4	1.132458e-4	0.04230
x	Biphenyl	1.660510e-12	1.660467e-12	6.941068e-7
massf	kg/h	158.68838	158.68838	0.00000
hflow	W	-2990.8	-2990.8	0.0

Stabilized liquid bottoms from the stripper column, free of light gases, fed to the benzene splitter.

StripperBtms

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	141.62	141.62	141.62
p	kPa	420.00	420.00	420.00
f	kmol/h	204.89	0.00	204.89
h	kJ/kmol	-16760.38	11232.84	-16760.38
s	kJ/kmol-K	-40.84	23.83	-40.84
hflow	W	-953875.7	0.0	-953875.7
x	Hydrogen	7.800531e-18	1.696046e-15	7.800531e-18
x	Methane	2.115100e-14	2.167573e-12	2.115100e-14
x	Benzene	0.76717	0.87612	0.76717
x	Toluene	0.21639	0.12362	0.21639
x	Biphenyl	0.01644	2.675539e-4	0.01644
massf	kg/h	16882.13555	0.00000	16882.13555
hflow	W	-953875.7	0.0	-953875.7

Feed stream to the benzene/toluene splitter column at column inlet conditions.

SplitterFeed

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	96.44	96.44	96.44
p	kPa	140.00	140.00	140.00
f	kmol/h	204.89	0.00	204.89
h	kJ/kmol	-24069.60	6561.71	-24069.60
s	kJ/kmol-K	-59.40	20.18	-59.40
hflow	W	-1369861.4	0.0	-1369861.4

x	Hydrogen	7.800531e-18	6.623120e-15	7.800531e-18
x	Methane	2.115100e-14	6.660897e-12	2.115100e-14
x	Benzene	0.76717	0.89347	0.76717
x	Toluene	0.21639	0.10643	0.21639
x	Biphenyl	0.01644	9.746255e-5	0.01644
massf	kg/h	16882.13555	0.00000	16882.13555
hflow	W	-1369861.4	0.0	-1369861.4

Distillation column separating high-purity benzene overhead from unreacted toluene .

Splitter							
Stage	T degC	P kPa	V kmol/h	L kmol/h	Q W	Feeds kmol/h	Draws kmol/h
1	88.21616	130.00000		159.39243	-2637418.51011		L 157.49445
2	88.44762	130.29412	316.88688	159.13010	0.00000		
3	88.71027	130.58824	316.62455	158.82260	0.00000		
4	89.00753	130.88235	316.31705	158.46711	0.00000		
5	89.34187	131.17647	315.96155	158.06299	0.00000		
6	89.71414	131.47059	315.55744	157.61262	0.00000		
7	90.12301	131.76471	315.10706	157.12190	0.00000		
8	90.56449	132.05882	314.61635	156.60037	0.00000		
9	91.03181	132.35294	314.09482	156.06068	0.00000		
10	91.51574	132.64706	313.55513	155.51742	0.00000		
11	92.00531	132.94118	313.01187	154.98559	0.00000		
12	92.48901	133.23529	312.48004	154.47889	0.00000		
13	92.95600	133.52941	311.97334	154.00837	0.00000		
14	93.39724	133.82353	311.50282	153.57745	0.00000		
15	93.80988	134.11765	311.07190	152.81877	0.00000		
16	94.52083	134.41176	310.31321	356.16309	0.00000	204.88508	
17	94.60238	134.70588	308.77245	356.21515	0.00000		
18	94.68679	135.00000	308.82452	356.25998	0.00000		
19	94.77715	135.29412	308.86935	356.29023	0.00000		
20	94.87970	135.58824	308.89960	356.29113	0.00000		
21	95.00695	135.88235	308.90050	356.23320	0.00000		
22	95.18393	136.17647	308.84257	356.05855	0.00000		

23	95.45993	136.47059	308.66792	355.65723	0.00000		
24	95.92908	136.76471	308.26660	354.83403	0.00000		
25	96.76088	137.05882	307.44340	353.28913	0.00000		
26	98.22538	137.35294	305.89850	350.69816	0.00000		
27	100.65250	137.64706	303.30752	347.02925	0.00000		
28	104.22203	137.94118	299.63861	342.97943	0.00000		
29	108.62982	138.23529	295.58880	339.79523	0.00000		
30	113.05781	138.52941	292.40460	338.21099	0.00000		
31	116.70265	138.82353	290.82035	337.91082	0.00000		
32	119.26252	139.11765	290.52019	338.17649	0.00000		
33	120.88200	139.41176	290.78586	338.47630	0.00000		
34	121.89870	139.70588	291.08567	335.63222	0.00000		
35	124.86995	140.00000	288.24159		2654218.40296		L 47.39063

Bottoms liquid from the splitter column consisting primarily of unreacted toluene.

SplitterBtms

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	124.87	124.87	124.87
p	kPa	140.00	140.00	140.00
f	kmol/h	47.39	0.00	47.39
h	kJ/kmol	-21764.93	11806.00	-21764.93
s	kJ/kmol-K	-48.10	32.71	-48.10
hflow	W	-286514.9	0.0	-286514.9
x	Hydrogen	2.334562e-25	1.248903e-22	2.334562e-25
x	Methane	3.580357e-25	1.248908e-22	3.580357e-25
x	Benzene	0.01000	0.02288	0.01000
x	Toluene	0.91893	0.97558	0.91893
x	Biphenyl	0.07107	1.541111e-3	0.07107
massf	kg/h	4568.90899	0.00000	4568.90899
hflow	W	-286514.9	0.0	-286514.9

Removes biphenyl from the recycled toluene.

biphenylCol

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Stage	T degC	P kPa	V kmol/h	L kmol/h	Q W	Feeds kmol/h	Draws kmol/h
1	110.19639	101.32500		44.53901	-825437.14696		L 44.02250
2	112.09270	101.32500	88.56151	85.53725	0.00000	47.39063	
3	121.09558	101.32500	82.16912	61.19496	0.00000		
4	191.40648	101.32500	57.82683	51.36548	0.00000		
5	242.76111	101.32500	47.99735		825881.25137		L 3.36813

Removed biphenyl

BiphenylPurge

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	242.76	242.76	242.76
p	kPa	101.33	101.33	101.33
f	kmol/h	3.37	0.00	3.37
h	kJ/kmol	204.33	45804.86	204.33
s	kJ/kmol-K	27.29	116.44	27.29
hflow	W	191.2	0.0	191.2
x	Hydrogen	6.492260e-25	7.509009e-22	6.492260e-25
x	Methane	1.245709e-24	7.507929e-22	1.245709e-24
x	Benzene	8.011528e-6	1.699908e-4	8.011528e-6
x	Toluene	0.01000	0.13378	0.01000
x	Biphenyl	0.98999	0.86605	0.98999
massf	kg/h	517.29943	0.00000	517.29943
hflow	W	191.2	0.0	191.2

Vapour purge stream taken from the recycle loop to prevent methane build-up in the system.

VapourPurge

Label	Unit	B	V	L
q	Fraction	1.00000	1.00000	0.00000
t	degC	35.00	35.00	35.00
p	kPa	3300.00	3300.00	3300.00
f	kmol/h	327.89	327.89	0.00
h	kJ/kmol	87.44	87.44	-30921.48
s	kJ/kmol-K	-22.37	-22.37	-81.89

hflow	W	7964.4	7964.4	0.0
x	Hydrogen	0.46264	0.46264	9.534707e-3
x	Methane	0.52916	0.52916	0.04200
x	Benzene	7.449836e-3	7.449836e-3	0.72775
x	Toluene	7.514106e-4	7.514106e-4	0.20514
x	Biphenyl	2.070978e-7	2.070978e-7	0.01558
massf	kg/h	3302.73238	3302.73238	0.00000
hflow	W	7964.4	7964.4	0.0

High-purity benzene product distillate recovered from the splitter column overhead.

SplitterOvhd

Label	Unit	B	V	L
q	Fraction	0.00000	1.00000	0.00000
t	degC	88.22	88.22	88.22
p	kPa	130.00	130.00	130.00
f	kmol/h	157.49	0.00	157.49
h	kJ/kmol	-24376.18	5558.95	-24376.18
s	kJ/kmol-K	-67.41	15.27	-67.41
hflow	W	-1066420.3	0.0	-1066420.3
x	Hydrogen	1.014797e-17	1.124307e-14	1.014797e-17
x	Methane	2.751541e-14	8.934435e-12	2.751541e-14
x	Benzene	0.99500	0.99794	0.99500
x	Toluene	5.000000e-3	2.056381e-3	5.000000e-3
x	Biphenyl	1.136052e-22	4.718539e-25	1.136052e-22
massf	kg/h	12313.22656	0.00000	12313.22656
hflow	W	-1066420.3	0.0	-1066420.3