

Example 4: Mass-Balance Only with Two Constraints/Targets (or Design-specs)

Let's add another design-spec to Example 3.

Notice that the mole fraction of CH₄ in Stream S6 is 29.85%. We like to fix this mole fraction at 35.0% as our second design-spec. It's obvious that the input parameter that most affects the mole fraction of methane in Stream S6 is the split fraction of methane in the separator, which at the moment is specified at 0.90 going to the overhead (S3). We will need a larger number in order obtain more methane in Stream S6.

Set up a second design-spec to:

1. Vary the split fraction of methane going to Stream S3 by specifying a range for A+ to adjust (0.90 – 0.99).
2. Specify the target to be the mole fraction of water in S4 being equal to 60%.
3. Specify the tolerance of the target (plus/minus).

Points to observe:

1. Notice that there are now 3 convergence loops, namely one for the tear stream and two for the two design-specs. However, the default convergence scheme in A+ will result in warnings. So we must converge all 3 loops simultaneously using Broyden.
2. The total number of iterations for the collapsed single loop using Broyden is 18.
3. The process feed flow (S1) was found to be 58.3853 lbmol/hr (DS-1), while the split fraction of methane going to Stream S3 was found to be 0.937369 (DS-2).

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___

Main Flowsheet x Control Panel x SEP (Sep) x **Convergence** x D

Tear Convergence Default Methods **Sequencing** Comments

Tearing and sequencing parameters

Design spec nesting **With Tears**

User nesting *Outside*

Variable weight 1

Loop weight 1

Tear Calculator export variables

Check sequence

Use affected block logic

Simulation Capital: ___USD Utilities: ___USD/Year Energy Savings: ___MW (___%)

Main Flowsheet x Control Panel x SEP (Sep) x Convergence x **DS-2 - Results** x Results S

Results **Status**

Variable	Initial value	Final value	Units
▶ MANIPULATED	0.9	0.937369	
▶ XCH4	0.377358	0.349999	

Main Flowsheet x Control Panel x SEP (Sep) x Convergence x Design Specs x Results Summary - Streams (All) x +

Clear Messages Check Status Run Settings Set Stop Points Convergence Monitor

Sequence Messages

Sequence:

- \$OLVER01
- REACTOR
- SEP
- SPLITTER

Flowsheet Analysis :

Block \$OLVER01 (Method: BROYDEN) has been defined to converge
streams: RECYCLE
specs : DS-1 DS-2

COMPUTATION ORDER FOR THE FLOWSHEET:
\$OLVER01 REACTOR SEP SPLITTER
(RETURN \$OLVER01)

->Calculations begin ...

		S1	S2	S3	S4	S6	RECYCLE
From			REACTOR	SEP	SEP	SPLITTER	SPLITTER
To		REACTOR	SEP	SPLITTER			REACTOR
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
Average MW		22.618092	22.930576	23.031208	22.40625	23.031208	23.031935
Mole Flows	lbmol/hr	58.385348	238.38535	200.00013	38.385218	20.000013	180
CH4	lbmol/hr	23.354139	74.677075	69.99994	4.6771348	6.999994	63.000005
O2	lbmol/hr	29.192674	5.8385348	0	5.8385348	0	0
CO2	lbmol/hr	0	80.552453	76.52483	4.0276226	7.652483	68.875383
H2O	lbmol/hr	0	23.782219	0.4756444	23.306575	0.0475644	0.4280799
H2	lbmol/hr	5.8385348	53.535066	52.999716	0.5353507	5.2999716	47.696532
Mole Fractions							
CH4		0.4	0.313262	0.3499995	0.1218473	0.3499995	0.35
O2		0.5	0.024492	0	0.1521037	0	0
CO2		0	0.3379086	0.3826239	0.1049264	0.3826239	0.382641
H2O		0	0.0997638	0.0023782	0.6071758	0.0023782	0.0023782
H2		0.1	0.2245736	0.2649984	0.0139468	0.2649984	0.2649807
Mass Flows	lb/hr	1320.5652	5466.3134	4606.2446	860.0688	460.62446	4145.7483