ADVANCE PVT LECTURE – 02

AGENDA:

1. Recap of Previous lecture
   - (a) Required parameters for EOS calculations
   - (b) How do we get these parameters
   - (c) Recap of Molar distb model
2. How TwoMw & Soreide param gives Mw & SG & how does Gamma param affect them?
3. Gamma distb model options in PhzComp
4. Why Lbc characterisation & Gamma charac are important
5. Using PhzComp to do Gamma fitting with different options and see the results

① RECAP OF LECTURE - 01

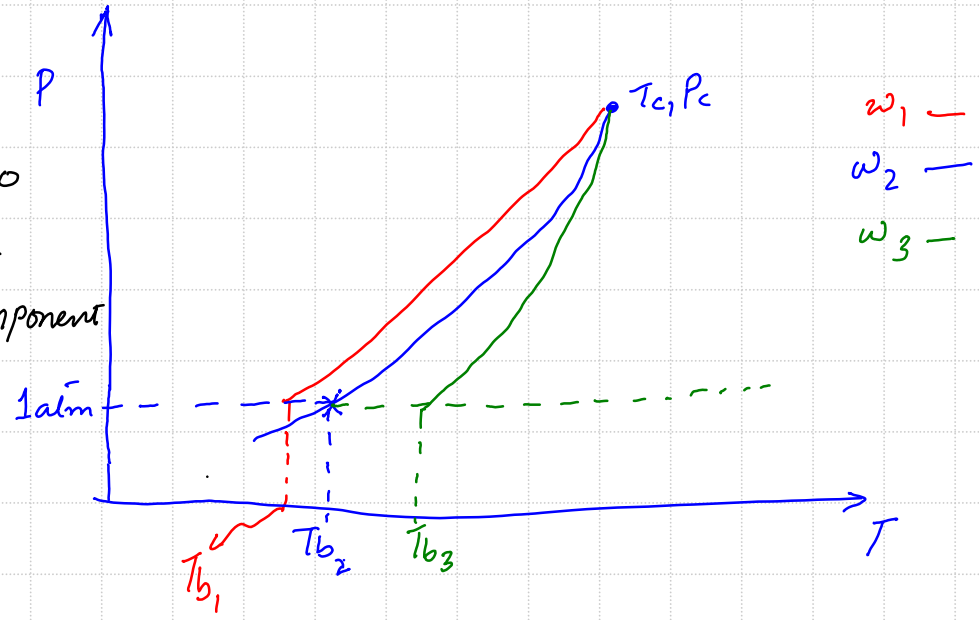
ⓐ EOS Calculations parameters:

① MW ⟶ we have Kalz Feroz, Twu MW correlation, Gamma distb model, Crude Assay data (measured data)

② T_c, P_c ⟶ Twu MW, $f(T_b)$: you need T_{bi}

③ ω (acentric factor)

determined in a manner so that T_c, P_c & T_b of the component are honored



④ s (volume shift)

Calculated so as to get correct 'SG' of each component: Need SG.

$(S.G)_{EOS}$ for component i = $(S.G)_{given}$ for comp i

⑤ molar composition

ⓐ user input

ⓑ molar distb models

MOLAR DISTB MODELS

(a) Exponential discrete
(b) Gamma continuous

(b) Gamma continuous:

(1) Shape, α
(2) bound, η
(3) Aug, M_{aug}

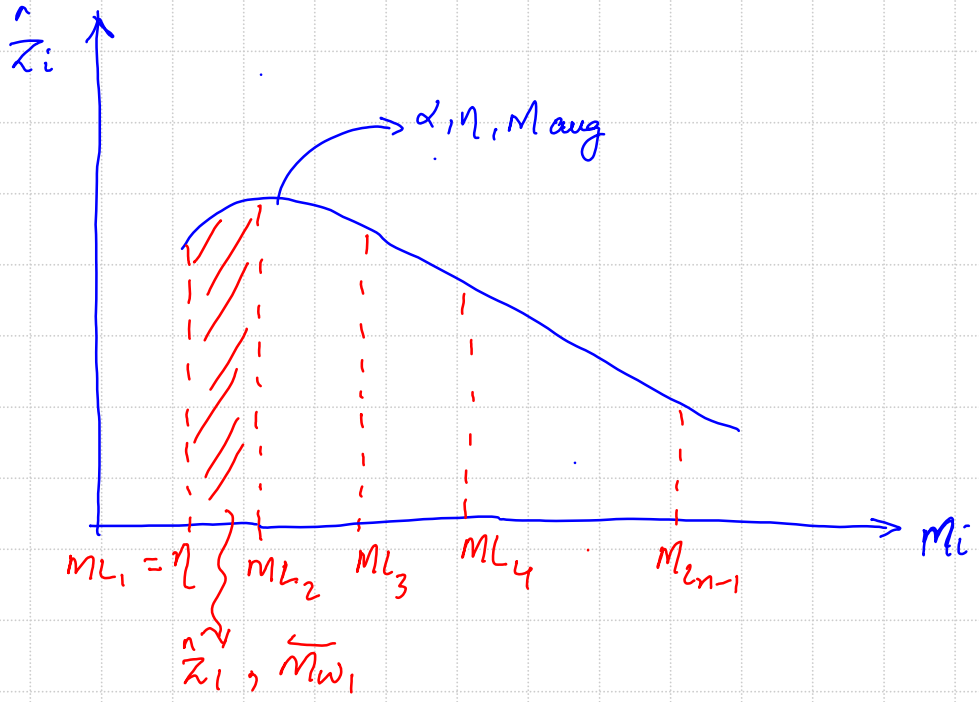
} defines the shape of distb model

(4) LMW's (lower MWs) → To discretize the Gamma model

Result

→ molar amounts of each component defined by LMWs

→ MW of each component



② TWUMW & SOREIDE : To get SG & MW

ⓐ Calculates properties for normal paraffins, $M_P, T_{cP}, P_{cP}, \gamma_P$. ($f(T_b)$ → of normal paraffin

ⓑ $\Delta\gamma = f(\gamma_{given} - \gamma_P)$, $f_T(\Delta\gamma, T_b)$

ⓒ T_c, P_c, M

In PhzComp

TWUMW keyword: value ranges 0 - 1

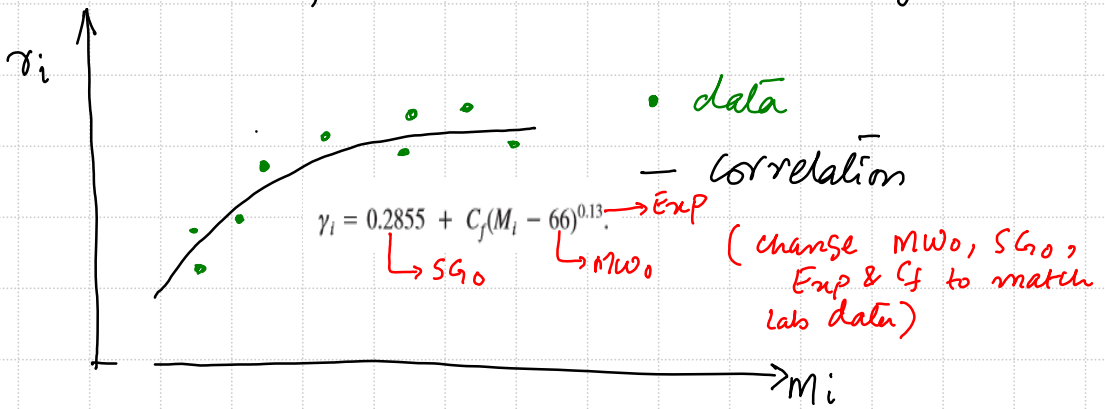
- If zero: dependency very small on $\Delta\gamma$
- If one: Full TWUMW correlation

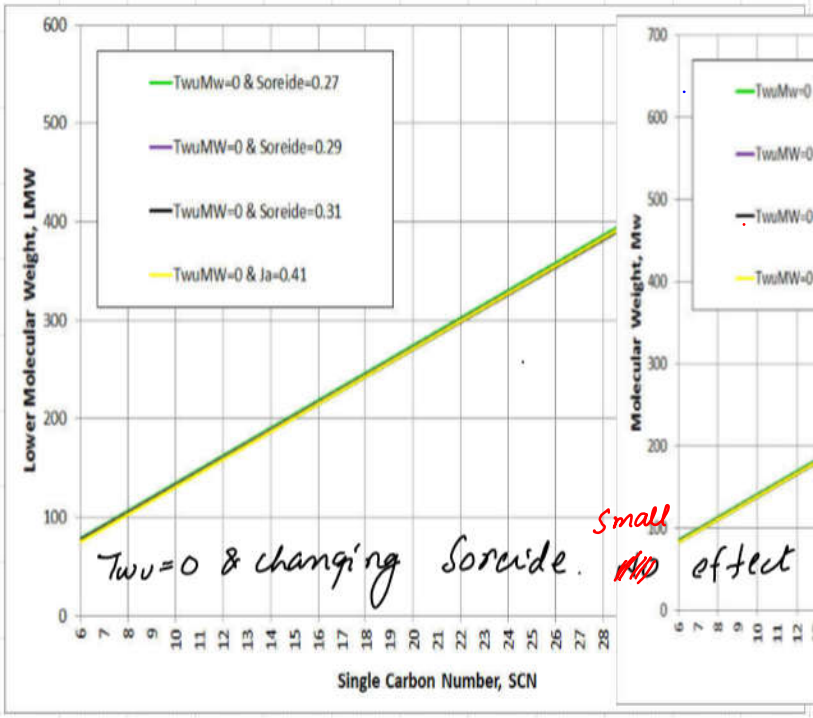
Soreide correlation (MW vs SG relationship)

→ gives SG based MWs

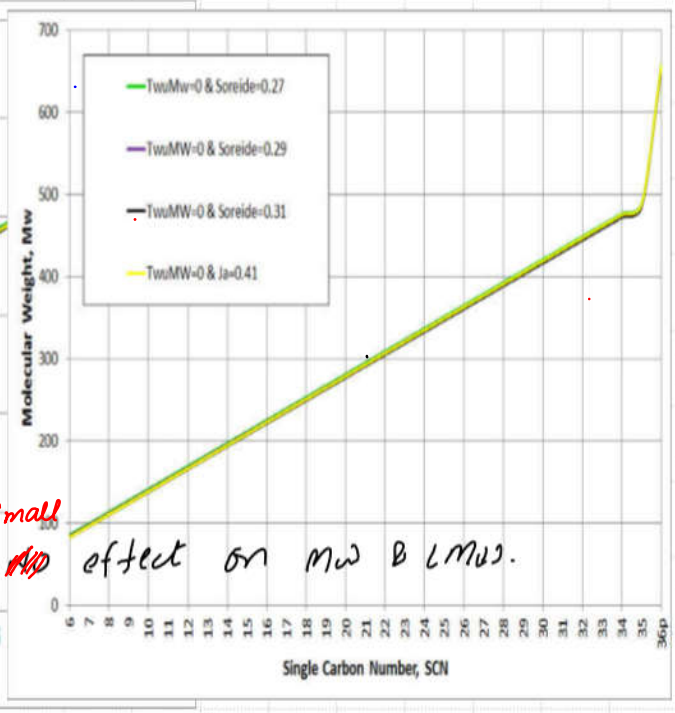
→ Different relationship for different type of fluids (how much aromatic, paraffinic

→ Normally you have reported M_{7+}, γ_{7+}, M_{n+}, γ_{n+} , M & r from Crude Assays

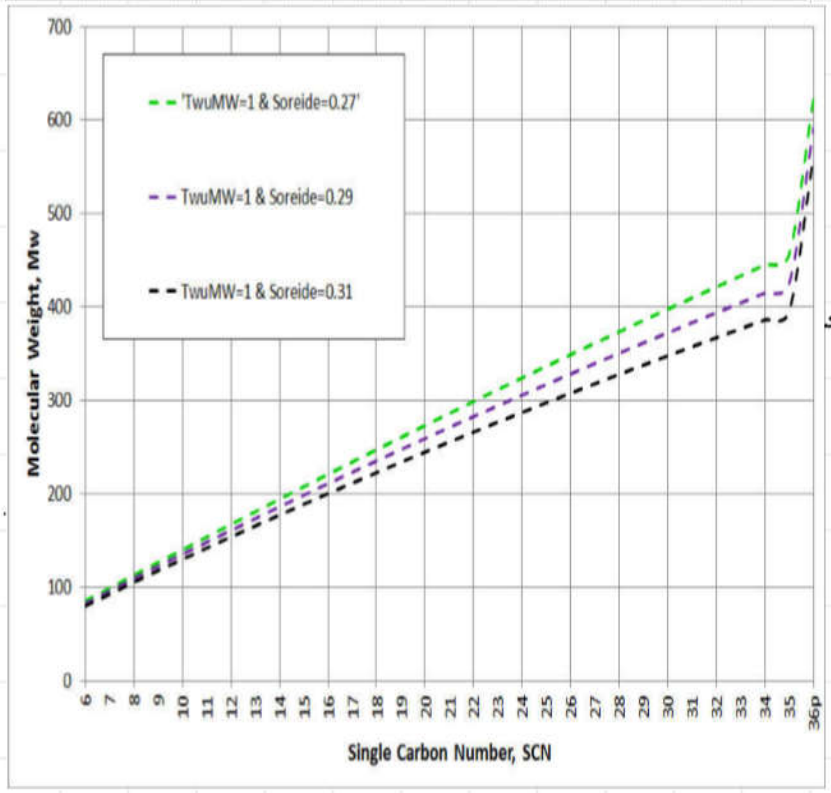




Twu=0 & changing Soreide.



Small effect on Mw & LMw.



⇒ Twu MW = 1 & changing Soreide. As Gf ↑ Mw ↓

Conclusion

① we need correct MW-SG relationship & Twu MW to get representative properties for EOS calculation

② Correct Twu MW is difficult to find as MW data is not usually measured on SCN basis: Potential Regression variable in tuning

Gamma modeling in PhzComp

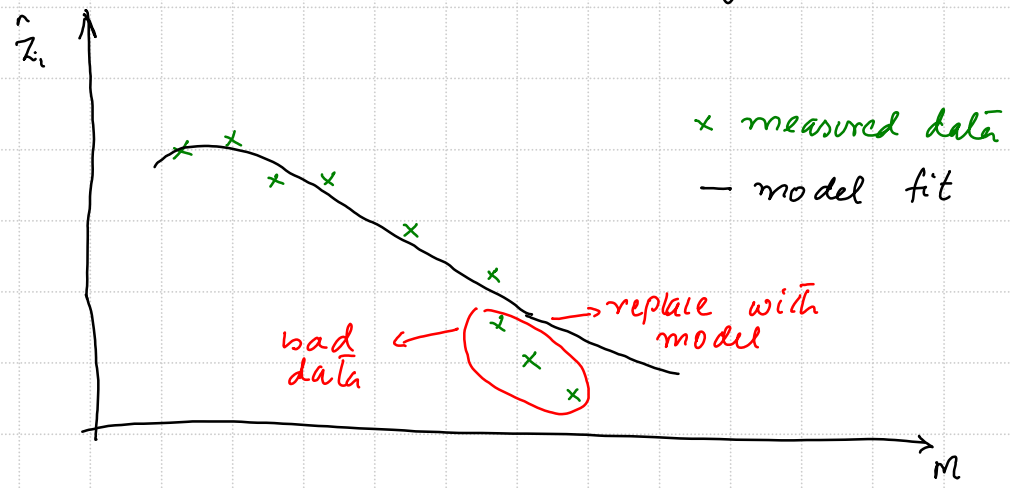
① Fitting Gamma model on reported composition

why do we need model when composition is available?

→ not all labs report the same heaviest fraction and same number of components

→ Single EOS has single definition of components so all streams should be splitted / lumped to EOS defined number of components using the fitted model

→ For QC & replacing bad measured data



② Splitting upto heaviest fraction of EOS charac for all samples.

GAMMA FITTING IN PHZ COMP

① Amount option

② MW option

① AMOUNT OPTION:-

ⓐ Min RMS b/w Calculated & reported amounts

ⓑ by changing α, η, Aug

ⓒ Need LMW's to be defined & composition to be fitted in

Final Result

→ Best fit α, η & Mavg

→ Mwi for each component

② MW option

① Min. RMS b/w Calculated & Reported MW's

② by changing η, Mavg, α

③ It calculates LMW's by matching the exact amounts

Result

→ Best fit α, η, Mavg

→ LMW's Specific for the Sample

→ Calculated Mwi for each component

Amount option	MW option
(+) matching measured data of mass amounts are matched	(−) Matching estimated MW's
(+) Fixed LMWs for all Samples giving correct amounts. BCZ EOS uses single set of LMWs based on which we will be splitting	(−) Variable LMW's that give correct amounts for each sample
(−) LMW need to be defined & should be consistent with MWs	(+) NO LMWs need to be defined

Conclusion:

Amount option with mass amounts being matched is the best option to use.

```
Conserve Mass
;Step 2: Defining LABSCN characterization for all samples and their respective feeds

CHAR       Dynamite-State-3975-16-21-1FH-LABSCN
EOS        PR79
Comp       Mw
H2S        34.080
N2         28.010
CO2        44.010
C1         16.040
C2         30.070
C3         44.100
I-C4       58.120
N-C4       58.120
I-C5       72.150
N-C5       72.150
C6         86.180
C7         92
C8         105
C9         119
C10        134
C11        147
C12        161
C13        175
C14        190
C15        206
C16        222
C17        237
C18        251
C19        263
C20        275
C21        291
C22        305
C23        318
C24        331
C25        345
C26        359
C27        374
C28        388
C29        402
C30p       527

END

Mix    Dynamite-State-3975-16-21-1FH-WellStream-LABSCN Moles  0.000  0.369  0.826  67.227  11.570  5.992  0.805  1.932  0.685  0.753  0.887
Mix    Dynamite-State-3975-16-21-1FH-SepOil-LABSCN     Moles  0.000  0.008  0.081   3.099   2.361  3.173  0.857  2.954  2.166  3.220  5.669
```

Conserve Mass → conserving mass so mass amounts measured in lab are honored everywhere.

① Lab charac includes component names the lab reports & lab reported MWs.

② Input lab feeds in mass if reported otherwise moles

③ If moles will be reported then lab MWs will be used to calculate lab measured mass amounts

④ If lab does not report MWs explicitly:

ⓐ lab MWs can be back calculated if wt% & mol% of any stream is given

ⓑ If that is not the case use Katz Ferozabadi MWs

```
TWUMW   0
Soreide
; Soreide parameters (best-fit to all data)
 SOREIDE
 MW0            66
 Exponent       0.13
 SG0            0.285
 Factor         0.29
```

→ Twu MW & Soreide will give MW & LMWs for Gamma charac in consistent way

```
;Defining new char for gamma fitting
CHAR    Dynamite-State-3975-16-21-1FH-Gamma-fit
EOS     PR79
Comp    Mw   LMW
H2S
N2
CO2
C1
C2
C3
```

From Twu MW & Soreide

```
Mix Dynamite-State-3975-16-21-1FH-WellStream-Gamma Dynamite-State-3975-16-21-1FH-WellStream-LABSCN 1 TANK
Mix Dynamite-State-3975-16-21-1FH-SepOil-Gamma Dynamite-State-3975-16-21-1FH-SepOil-LABSCN 1 TANK
```

→ Importing feeds in new charac with conserved mass so lab measured mass will be conserved & moles will change based on new MW's

Q Why Gamma charac is needed? Why cant we use lab charac for Gamma fitting?

As discussed earlier that for amount option we need LMWs to be defined. In lab charac since MWs are the most important to get the correct masses from modes so if we try to input LMW's by ourselves in lab charac then PhzComp will give error that MW & LMW are not consistent. If we try to estimate LMWs from TwoMW correlation against given MWs then we can get consistent LMWs for given MWs but the problem is these LMWs will be different for different samples (lab characterizations). So during Gamma fitting different set of LMWs will be used for different samples while when we will be splitting them in EOS charac then we will have single set of LMW's. So this does not bring consistency.

So Gamma charac is required:

(a) to have consistent MWs & LMWs definition for gamma fitting

(b) to ensure same LMWs used for γ-fitting for all samples and should have same LMWs in EOS charac for splitting.

Notes: Even though Gamma charac will be different for different samples (if samples have different heaviest fraction definition) but MWs & LMWs will be same in all including EOS charac bcz we are using same TwoMW & Soreide for all of them.

Q Importance of Gamma charac for MW option?

No need of Gamma charac for MW option as we dont need any lmws

```
Gamma
split C7 → using γ-model for C7+ fractions
Shape 1 0.5 3
Average 183 170 200   } variables
Bound 90 80 100
Fit Dynamite-State-3975-16-21-1FH-SepOil-Gamma C7 amount → Mass amounts will be fitted
Store Dynamite-State-3975-16-21-1FH-SepOil-Gamma-fit-param → storing best fit γ-parameters
End
```

(→ Fitting to C7+ fractions; → amount option)

Instead of amount MW option can also be used. If we want to ignore all components above a certain component like C_{20} then we write 'Ignore C20' after Fit Commands

If we want to change weight factor of certain components write "WT 'component name' 'number'" after fit command

PHAZCOMP CALCULATIONS WITH AMOUNT OPTION:

Component	Mol Wt	
H2S	34.080	34.082
N2	28.010	28.014
CO2	44.010	44.010
C1	16.040	16.043
C2	30.070	30.070
C3	44.100	44.097
I-C4	58.120	58.123
N-C4	58.120	58.123
I-C5	72.150	72.150
N-C5	72.150	72.150
C6	86.180	84.043
C7	92.000	97.812
C8	105.000	111.749
C9	119.000	125.727
C10	134.000	139.716
C11	147.000	153.705
C12	161.000	167.690
C13	175.000	181.672
C14	190.000	195.649
C15	206.000	209.622
C16	222.000	223.591
C17	237.000	237.557
C18	251.000	251.520
C19	263.000	265.481
C20	275.000	279.440
C21	291.000	293.398
C22	305.000	307.354
C23	318.000	321.309
C24	331.000	335.263
C25	345.000	349.217
C26	359.000	363.170
C27	374.000	377.123
C28	388.000	391.077
C29	402.000	405.030
C30p	527.000	418.984

→ Column 1 mws are the ones lab is using

→ Column 2 mws are the ones calculated by TwuMW used in Gamma charac

values slightly different

→ very large difference. TwuMW correlation does not recognize C30p. It recognizes C30 (ignoring 'p') and gives C30 mol. wt which is wrong. So in Gamma charac MW C30p is wrong.

Q Does this wrong MW makes any difference to Gamma fitting?

For the amount option it does not make any difference as we have conserved mass and feed in Gamma charac contains correct masses which we are fitting The wrong MW will give us wrong moles of C30p using Lab mass but we are fitting mass and not moles.

For MW option, if we are using Gamma Charac then we will have to ignore C30p in fitting as its MW is wrong and we dont want it in regression. If we are using lab charac for fitting with MW option then no need to ignore this component as MW inputted is correct

Note If we are using multiple samples in Lab Charac and has defined MWnt = 1 and defining Cnt mass by using multiply commands then we also will have to ignore C30p MW even though we are using Lab charac for fitting.

Component	Moles	Mole Fracs		Mass	Mass Fracs	
H2S	0.0000	0.00000	0.000000	0.000	0.000	0.000000
N2	0.3690	0.36895	0.003690	10.336	10.336	0.002799
CO2	0.8260	0.82600	0.008260	36.352	36.352	0.009846
C1	67.2270	67.21443	0.672263	1078.321	1078.321	0.292064
C2	11.5700	11.57000	0.115699	347.910	347.910	0.094231
C3	5.9920	5.99241	0.059919	264.247	264.247	0.071571
I-C4	0.8050	0.80496	0.008050	46.787	46.787	0.012672
N-C4	1.9320	1.93190	0.019320	112.288	112.288	0.030413
I-C5	0.6850	0.68500	0.006850	49.423	49.423	0.013386
N-C5	0.7530	0.75300	0.007530	54.329	54.329	0.014715
C6	0.8870	0.90956	0.008870	76.442	76.442	0.020704
C7	1.3120	1.23403	0.013120	120.704	120.704	0.032693
C8	1.5440	1.45075	0.015440	162.120	162.120	0.043910
C9	0.9850	0.93230	0.009850	117.215	117.215	0.031748
C10	0.7450	0.71452	0.007450	99.830	99.830	0.027039
C11	0.5360	0.51262	0.005360	78.792	78.792	0.021341
C12	0.4350	0.41765	0.004350	70.035	70.035	0.018969
C13	0.4270	0.41132	0.004270	74.725	74.725	0.020239
C14	0.3590	0.34864	0.003590	68.210	68.210	0.018475
C15	0.3300	0.32430	0.003300	67.980	67.980	0.018412
C16	0.2610	0.25914	0.002610	57.942	57.942	0.015694
C17	0.2360	0.23545	0.002360	55.932	55.932	0.015149
C18	0.2280	0.22753	0.002280	57.228	57.228	0.015500
C19	0.1840	0.18228	0.001840	48.392	48.392	0.013107
C20	0.1430	0.14073	0.001430	39.325	39.325	0.010651
C21	0.1330	0.13191	0.001330	38.703	38.703	0.010483
C22	0.1130	0.11213	0.001130	34.465	34.465	0.009335
C23	0.0990	0.09798	0.000990	31.482	31.482	0.008527
C24	0.0970	0.09577	0.000970	32.107	32.107	0.008696
C25	0.0870	0.08595	0.000870	30.015	30.015	0.008130
C26	0.0770	0.07612	0.000770	27.643	27.643	0.007487
C27	0.0690	0.06843	0.000690	25.806	25.806	0.006990
C28	0.0620	0.06151	0.000620	24.056	24.056	0.006516
C29	0.0550	0.05459	0.000550	22.110	22.110	0.005988
C30p	0.4380	0.55092	0.004380	230.826	230.826	0.062519
Totals:	100.0010	1.000000		3692.077	1.000000	

moles in lab charac } ≠ { moles in Gamma charac

mass amounts in tank defined in lab charac } = { mass amounts in tank defined in Gamma charac.

Always compare mass and moles and not the fraction amounts.

Component	Mol Wt	LMW	
H2S	34.082		
N2	28.014		
CO2	44.010		
C1	16.043		
C2	30.070		
C3	44.097		
I-C4	58.123		
N-C4	58.123		
I-C5	72.150		
N-C5	72.150		
C6	84.043	77.029	
C7	97.812	90.799	97.81
C8	111.749	104.735	104.74
C9	125.727	118.714	118.71
C10	139.716	132.702	132.70
C11	153.705	146.691	146.69
C12	167.690	160.677	160.68
C13	181.672	174.658	174.66
C14	195.649	188.635	188.64
C15	209.622	202.608	202.61
C16	223.591	216.578	216.58
C17	237.557	230.544	230.54
C18	251.520	244.507	244.51
C19	265.481	258.468	258.47
C20	279.440	272.427	272.43
C21	293.398	286.384	286.38
C22	307.354	300.340	300.34
C23	321.309	314.295	314.30
C24	335.263	328.249	328.25
C25	349.217	342.203	342.20
C26	363.170	356.157	356.16
C27	377.123	370.110	370.11
C28	391.077	384.063	384.06
C29	405.030	398.017	398.02
C30p	418.984	411.971	411.97

LMWs calc in Gamma charac by Twu Mw & Soreide

MWs taken from Gamma fit Results table both exactly same (second ones are round off to two decimal places) except C7 LMW. Because C7 LMW has to be equal to calculated 'η' during fitting

Shape Parameter (Alpha) ... :	0.69580	Beta Parameter .... :	133.534
Average MW Multiplier ..... :	1.01815	Average Plus MW ... :	190.726
Bounding MW Multiplier .... :	1.00000	Bounding MW ..... :	97.812
Origin MW Multiplier ..... :	1.00000	Origin MW ..... :	97.812
Number of Iterations ..... :	4	RMS % Error ..... :	0.361

variables

RMS reduced b/w these two

Component	Lower MW	Reported MW	Calculated MW	Reported Moles	Calculated Moles	Reported Mass	Calculated Mass	Percent Deviation	Relative Weight
C7	97.81	97.81	100.62	0.127900	0.135105	0.066783	0.072570	0.58	1.00
C8	104.74	111.75	111.22	0.163798	0.144373	0.097713	0.085719	-1.20	1.00
C9	118.71	125.73	125.41	0.107599	0.103662	0.072217	0.069397	-0.28	1.00
C10	132.70	139.72	139.46	0.083527	0.082262	0.062297	0.061240	-0.11	1.00
C11	146.69	153.70	153.47	0.060309	0.067778	0.049485	0.055529	0.60	1.00
C12	160.68	167.69	167.47	0.049156	0.056983	0.044004	0.050944	0.69	1.00
C13	174.66	181.67	181.47	0.048350	0.048520	0.046890	0.047002	0.01	1.00
C14	188.64	195.65	195.45	0.040991	0.041677	0.042812	0.043484	0.07	1.00
C15	202.61	209.62	209.43	0.038105	0.036029	0.042640	0.040279	-0.24	1.00
C16	216.58	223.59	223.40	0.030506	0.031299	0.036412	0.037326	0.09	1.00
C17	230.54	237.56	237.37	0.027748	0.027295	0.035189	0.034586	-0.06	1.00
C18	244.51	251.52	251.33	0.026792	0.023877	0.035973	0.032036	-0.39	1.00
C19	258.47	265.48	265.30	0.021413	0.020942	0.030346	0.029659	-0.07	1.00
C20	272.43	279.44	279.26	0.016558	0.018407	0.024699	0.027441	0.27	1.00
C21	286.38	293.40	293.22	0.015543	0.016209	0.024344	0.025372	0.10	1.00
C22	300.34	307.35	307.17	0.013248	0.014296	0.021736	0.023443	0.17	1.00
C23	314.30	321.31	321.13	0.011499	0.012627	0.019724	0.021646	0.19	1.00
C24	328.25	335.26	335.08	0.011326	0.011166	0.020270	0.019973	-0.03	1.00
C25	342.20	349.22	349.04	0.010074	0.009884	0.018780	0.018417	-0.04	1.00
C26	356.16	363.17	362.99	0.008979	0.008758	0.017408	0.016971	-0.04	1.00
C27	370.11	377.12	376.95	0.008103	0.007767	0.016313	0.015629	-0.07	1.00
C28	384.06	391.08	390.90	0.007255	0.006893	0.015145	0.014385	-0.08	1.00
C29	398.02	405.03	404.86	0.006419	0.006122	0.013878	0.013232	-0.06	1.00
C30p	411.97	418.98	535.83	0.064803	0.050245	0.144943	0.143721	-0.12	1.00
Totals	97.81	187.33	190.73	1.000000	0.982178	1.000000	1.000000	1.81*	0.00*

Same from Gamma charac

From Gamma charac

From r-chara

From calc mass & calc. MWs

MWs from best fit Gamma model & LMWs provided

weight factors for each component

418 is MW C30p calculated by TwoMW considering it C30 however 535 is MW calculated by Gamma model by integrating from LMW of C30p to infinity. So 535 is correct/representative MW of C30p rather than 418.

So Gamma model is needed to get the correct MW of Cn+ which cannot be obtained from TwoMW alone

AC of Gamma fitting can be done:

(a) by visualizing the fitting results in a plot

(b) looking at over all RMS

(c) Calculated Mavg Plus ±10% of lab value

(d) calculated MW of Cn+ ±10% of lab value

PHAZCOMP CALCULATIONS WITH MW OPTION:

Everything is same until Gamma fit Results which are shown below:

Shape Parameter (Alpha) ... :	0.69554	Beta Parameter .... :	135.350
Average MW Multiplier .... :	1.01574	Average Plus MW ... :	190.441
Bounding MW Multiplier .... :	0.98104	Bounding MW ..... :	96.300
Origin MW Multiplier ..... :	1.00000	Origin MW ..... :	96.300
Number of Iterations ..... :	4	RMS % Error ..... :	0.578

variables

min RMS b/w two

Component	Reported Mass	Calculated Mass	Reported Moles	Calculated Moles	Lower MW	Reported MW	Calculated MW	Percent Deviation	Relative Weight	
C7	0.066783	0.066783	0.127557	0.126650	96.30	91.148	98.16	98.86	0.72	1.00
C8	0.097713	0.097713	0.163666	0.166408	102.61	104.923	111.94	110.09	-1.65	1.00
C9	0.072217	0.072217	0.107581	0.107353	118.91	118.844	125.86	126.12	0.21	1.00
C10	0.062297	0.062297	0.083539	0.082770	134.01	132.804	139.82	141.12	0.93	1.00
C11	0.049485	0.049485	0.060330	0.059869	148.74	146.772	153.79	154.97	0.77	1.00
C12	0.044004	0.044004	0.049180	0.049245	161.55	160.741	167.75	167.53	-0.13	1.00
C13	0.046890	0.046890	0.048379	0.048662	173.81	174.707	181.72	180.66	-0.58	1.00
C14	0.042812	0.042812	0.041020	0.041241	187.88	188.668	195.68	194.63	-0.54	1.00
C15	0.042640	0.042640	0.038135	0.038255	201.72	202.624	209.64	208.98	-0.31	1.00
C16	0.036412	0.036412	0.030533	0.030571	216.61	216.576	223.59	223.31	-0.12	1.00
C17	0.035189	0.035189	0.027775	0.027802	230.32	230.525	237.54	237.30	-0.10	1.00
C18	0.035973	0.035973	0.026819	0.026731	244.60	244.470	251.48	252.32	0.33	1.00
C19	0.030346	0.030346	0.021436	0.021270	260.42	258.412	265.43	267.50	0.78	1.00
C20	0.024699	0.024699	0.016576	0.016472	274.90	272.351	279.36	281.13	0.63	1.00
C21	0.024344	0.024344	0.015562	0.015515	287.60	286.289	293.30	294.19	0.30	1.00
C22	0.021736	0.021736	0.013264	0.013258	301.05	300.225	307.24	307.38	0.05	1.00
C23	0.019724	0.019724	0.011514	0.011551	313.96	314.160	321.17	320.14	-0.32	1.00
C24	0.020270	0.020270	0.011341	0.011399	326.56	328.094	335.11	333.39	-0.51	1.00
C25	0.018780	0.018780	0.010088	0.010137	340.50	342.027	349.04	347.36	-0.48	1.00
C26	0.017408	0.017408	0.008992	0.009031	354.49	355.959	362.97	361.38	-0.44	1.00
C27	0.016313	0.016313	0.008115	0.008144	368.55	369.892	376.91	375.55	-0.36	1.00
C28	0.015145	0.015145	0.007265	0.007283	382.85	383.824	390.84	389.92	-0.23	1.00
C29	0.013878	0.013878	0.006428	0.006435	397.29	397.756	404.77	404.34	-0.11	1.00
C30p	0.144943	0.148308	0.064904	0.051765	411.69	411.689	418.70	537.16	28.29	0.00
Totals	1.000000	1.003365	1.000000	0.987818	96.30	187.49	190.44	1.57	0.00	

w1=0 ignore

mass amounts are exactly matched except for C30p by changing LMWs

Mass amounts are matched bc2 mass is conserved

LMWs calculated so to match mass amounts ≠ LMWs from r-charac

↓

will vary from sample to sample therefore MW option does not ensure fitting based on common LMWs

Representative MW of C30p from Gamma mode

MW C30p from Gamma charac was wrong so C30p has to be ignored

↓

no need to ignore if MW of C30p would be correct (if lab charac was used for fitting)