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Peng-Robinson Equation of State Predictions for Gas Condensate Before and After Lumping

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Abstract

Gas condensate compositional simulation studies are conducted to evaluate gas and condensate reserves and make comparisons of production methods for the economic development of a reservoir. The data needed for the evaluation are dew point pressure, gas compressibility factor, liquid volume and produced gas. Hosein and Dawe showed that compositional analysis greater than Single Carbon Number 24 (SCN24) is required for accurate prediction of these data by a tuned Equation of State (EOS). However they did not demonstrate the accuracy of their tuning technique with lumped components which are applied when performing simulation studies to reduce cost and computer time involved.

Simple and complex schemes for lumping of the SCN groups into less than 6 Multiple Carbon Number (MCN) groups have been devised. However there are currently no criteria for selecting the best lumping scheme that will give similar accuracy to using many SCN groups except by trial and error, or by algorithms designed to test a number of schemes and to select the best one. In this paper we have used Whitson's lumping scheme which is in the form of a simple mathematical expression in comparison to other lumping schemes from the open literature.

The tuning technique of Hosein and Dawe was applied and differences of less than ±4.0 % from tuned EOS predictions before and after lumping of the SCN groups were obtained. These results indicate that the tuning technique of Hosein and Dawe could be used to perform accurate simulation studies of lean and rich gas condensate systems using MCN groups lumped by the Whitson's lumping scheme. Complex algorithms are not necessary to select an appropriate lumping scheme.

Key words: Gas condensate; Equation of state; Predictions; Single carbon number; Lumping

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INTRODUCTION

Gas condensate field development planning requires compositional simulation studies using a tuned Equation of State (EOS) for the evaluation of gas and condensate reserves, production methods, facilities design as well as economic development (Coats et al 1986; Pedersen et al 1989; Danesh 1998). The physical property data needed for such evaluation are dew point pressure, gas compressibility factor, liquid volume and produced gas (Constant Volume Depletion, CVD data) which are predicted by the tuned Equation of State (EOS). EOS tuning techniques for accurate prediction have been studied (Coats et al 1986; Pedersen et al 1989; Danesh 1998; Hosein 2004). Recently Hosein and Dawe (2011) showed that tuning of the EOS constants called the omegas, Ω's (Ω_a and Ω_b of methane and Ω_a and Ω_b of the plus fraction) can give a more accurate prediction than tuning the critical pressure (P_c), critical temperature (T_c) and acentric factor (ω) of the plus fraction and the Volume Shift Parameter (VSP). For the Peng-Robinson (1976) EOS, Ω_a and Ω_b take the values of 0.45724 and 0.07780 at the critical point (Soave 1972; Martin 1979).

The data required for the physical property prediction by any EOS are pressure, temperature and composition. The composition of a sample is experimentally determined

by gas chromatography and components heavier than pentanes are lumped into Single Carbon Number (SCN) groups (Katz and Firoozabadi 1978; Pedersen 1989; Hosein 2004; Hosein and Dawe 2011). The last group is known as the plus (C_+) or last fraction. Prior to tuning, the number of SCN (Single Carbon Number) groups required to converge the EOS predicted values to the experimentally measured values is determined (Pedersen et al 1989; Danesh 1998). Often extended analysis of the plus fraction (Pedersen 1989; Al-Meshari and McCain 2007; Hosein and McCain 2009) is needed for this step. Studies have shown that after performing this step, minimal tuning of the EOS parameters is required (Pedersen et al 1989; Danesh 1998; Hosein 2004). Hosein and Dawe (2011) recently demonstrated accurate predictions with compositions up to SCN24 and beyond after tuning the Peng-Robinson (1976) EOS. However in order to reduce simulation costs and computing time, lumping schemes (Whitson 1980, Behrens and Sandler 1986; Ahmed 1989; Pedersen et al 1989; Danesh 1998) to reduce the number of SCN groups into three to five Multiple Carbon Number (MCN) groups (pseudo-components) are used.

The number of MCN groups required and the distribution of SCN groups within each MCN group can be calculated by a simple form (e.g. Whitson 1980) or more complex lumping forms (e.g. Behrens and Sandler 1986) of the SCN groups. Currently there are no standard criteria for selecting the best lumping scheme to give similar accuracy as can be calculated by the many SCN groups, except by trial and error or by algorithms (Danesh 1998; Kai 2001) designed to test a number of schemes. The best one is then selected.

In this study we use the Whitson (1980) lumping scheme to demonstrate that the tuning technique of Hosein and Dawe (2011) gives minimal differences before and after lumping for a lean and a rich gas condensate sample. Hence complex algorithms are not necessary to select an appropriate lumping scheme.

1. WHITSON'S (1980) LUMPING SCHEME

Whitson's (1980) lumping scheme involves two calculation steps which can be performed by a hand held calculator.

Step 1: The numbers of MCN groups are determined as follows:

$$N_g = \text{Integer}\,[1 + 3.3\ \text{Log}\,(N - n)] \quad (1)$$

where N_g=number of Multiple Carbon Number (MCN) groups

n=number of carbon atoms of the first heavy SCN group (i.e. 7 for this study)

N=number of carbon atoms of the plus (last) fraction (i.e. 25 for this study)

Step 2: The distribution of SCN groups within each MCN group are determined from molecular weights as follows:

$$(M)_I = (M)_n\,[\text{Exp.}\,\{(1 / N_g)\ \text{Ln.}\,((M)N / (M)_n)\}]^I \quad (2)$$

where $(M)_n$=molecular weight of the first heavy SCN group (i.e.SCN7)

$(M)_N$=molecular weight of the plus (last) fraction

I=1, 2, ….., N_g.

A sample calculation using Whitson (1980) lumping Scheme for Trinidad Sample A is given in the Appendix.

2. THERMODYNAMIC MODEL AND FLUID SYSTEM

2.1 Sample Compositions and Physical Properties

The compositions of the two samples (Hosein and Dawe 2011; Whitson and Torp 1983) studied, A and B, are given in Table 1. The first heavy group is SCN7 and the plus (or last) fraction is the C_{25+}. The physical properties for the SCN groups and the plus fractions were also included in Table 1 (Hosein and Dawe 2011; Whitson and Torp 1983). Sample A is a lean gas condensate (mole % of $C_{7+} \leq 4$ %, McCain 1999) from offshore Trinidad that was used to demonstrate the tuning technique with the omegas, Ω's (Hosein and Dawe 2011). Sample B is a rich gas condensate sample from the North Sea (Whitson and Torp 1983). It was included in this study to demonstrate that the tuning technique of Hosein and Dawe (2011) can be applied to gas condensate samples from regions other than Trinidad.

Table 1
Compositions and Properties for Trinidad Sample A and North Sea Sample B. Data taken from Hosein and Dawe (2011) and Whitson and Torp (1983)

Component	Symbol	Sample A	Sample B	Specific	Molecular
		Mole %	Mole %	Gravity	Wt., g/mol
Carbon dioxide	CO_2	0.350	2.370	0.817	44
Nitrogen	N_2	0.077	0.310	0.809	28
Methane	C_1	91.890	73.190	0.300	16
Ethane	C_2	1.826	7.800	0.356	30
Propane	C_3	1.212	3.550	0.507	44
iso-Butane	i-C_4	0.383	0.710	0.563	58
n-Butane	n-C_4	0.500	1.450	0.584	58
iso-Pentane	i-C_5	0.241	0.640	0.624	72
n-Pentane	n-C_5	0.216	0.680	0.631	72
Hexanes	SCN6	0.386	1.090	0.685	84
Heptanes	SCN7	0.508	1.214	0.722	96
Octanes	SCN8	0.652	1.173	0.745	107
Nonanes	SCN9	0.353	0.860	0.764	121
Decanes	SCN10	0.286	0.687	0.778	134
Undecanes	SCN11	0.194	0.568	0.789	147
Dodecanes	SCN12	0.134	0.478	0.800	161
Tridecanes	SCN13	0.146	0.407	0.811	175
Tetradecanes	SCN14	0.121	0.350	0.822	190
Pentadecanes	SCN15	0.103	0.302	0.832	206
Hexadecanes	SCN16	0.077	0.262	0.839	222
Heptadecanes	SCN17	0.065	0.228	0.847	237
Octadecanes	SCN18	0.052	0.199	0.852	251
Nonadecanes	SCN19	0.041	0.174	0.857	263
Eicosanes	SCN20	0.035	0.153	0.862	275

To be continued

Continued

Component	Symbol	Sample A	Sample B	Specific	Molecular
		Mole %	Mole %	Gravity	Wt., g/mol
Heneicosanes	SCN21	0.030	0.134	0.867	291
Docosanes	SCN22	0.024	0.118	0.872	305
Tricosanes	SCN23	0.019	0.104	0.877	318
Tetracosanes	SCN24	0.015	0.092	0.881	331
Heptanes plus	C_{7+}	2.919	-	0.794	150
Pentacosanes plus	C_{25+}	0.098	-	0.893	398
Heptanes plus	C_{7+}	-	8.210	0.816	184
Pentacosanes plus	C_{25+}	-	0.903	0.919	462

2.2 Tuning of the Peng-Robinson (1976) EOS before Lumping

Hosein and Dawe's (2011) tuning technique with the Peng-Robinson (1976) EOS was applied using the CMG (Computer Modeling Group) software (WINPROP 2002) to predict dew point pressure (DPP), gas compressibility factor (Z factor), liquid volume (LDO) and produced gas (PG). The data input into the software for the calculations were the sample compositions given in Table 1, reservoirs temperatures (186 °F for sample A and 280 °F for sample B) and the depletion pressures given in Tables 4 and 6 (first column) for sample A and Tables 5 and 7 (first column) for sample B. The tuning parameters of binary interaction coefficient, BIC (interaction between pairs of molecules of different sizes in a mixture) (Soave 1972; Oellrich et al 1981) between methane and the heavy fractions (greater than SCN6 and including the plus fraction), Ω_a and Ω_b for methane and Ω_a and Ω_b for the plus (last) fraction were adjusted as a group (Agarwal et. al. 1990) to reduce the objective function F to a minimum (Dennis et. al., 1981), as follows:

$$F = \sum_{i}^{N} [wi\ (y_{i,\ pred.} - y_{i,\ expt.}) / y_{i,\ expt.}]^2 \quad (3)$$

where $y_{i,pred.}$ and $y_{i,expt.}$ correspond to the predicted (before lumping) and experimental data shown in Tables 3, 4 and 5 .

The weight factors, w_i (Agarwal et. al. 1990) applied to the experimental data were 40 for dew point pressure (Coats et. al. 1986), 1 for liquid volume and 10 for gas compressibility factor (Hosein and Dawe 2011). These weight factors for liquid volume and gas compressibility factor were determined by Hosein and Dawe (2011) in their tuning study with the Ω's, from which they obtained differences of less than ±8.0 % between the predicted and experimental data for compositional analyses to SCN24 and beyond. In this study compositional analysis to SCN 24 were used in the predictions by the Peng-Robinson (1976) EOS before lumping.

2.3 Lumping of SCN Groups

The compositional and physical properties for samples A and B in Table1 were applied with the Whitson's (1980) lumping scheme. The 18 SCN groups (SCN7 to SCN24 inclusive) and the plus fraction (C_{25+}) were reduced to the 5 MCN groups given in Table 2 after lumping (see Appendix for sample calculation). The distribution of SCN groups in each MCN group (see Appendix) is also included in Table 2. The mole % of each MCN group is the sum of the mole % of the SCN groups distributed in each MCN group (Whitson 1980; Ahmed 1989). The physical properties of the MCN groups given in Table 2 were calculated by the software (WINPROP 2002) using the mixing rules of Lee and Kesler (1975).

Table 2
Compositions and Properties for Trinidad Sample A and North Sea Sample B after Lumping with Whitson (1980) Lumping Scheme

Component	Symbol	Sample A	Specific	Molecular
		Mole %	Gravity	Wt., g/mol
Carbon dioxide	CO_2	0.350	0.817	44
Nitrogen	N_2	0.077	0.809	28
Methane	C_1	91.890	0.300	16
Ethane	C_2	1.826	0.356	30
Propane	C_3	1.212	0.507	44
iso-Butane	i-C_4	0.383	0.563	58
n-Butane	n-C_4	0.500	0.584	58
iso-Pentane	i-C_5	0.241	0.624	72
n-Pentane	n-C_5	0.216	0.631	72
Hexanes	SCN6	0.386	0.685	84
SCN7 to SCN9	MCN1	1.513	0.747	106
SCN10 to SCN12	MCN2	0.614	0.791	144
SCN13 to SCN16	MCN3	0.447	0.828	194
SCN17 to SCN21	MCN4	0.223	0.859	258
SCN22 to $C2_{5+}$	MCN5	0.122	0.888	356
Component	Symbol	Sample B	Specific	Molecular
		Mole %	Gravity	Wt., g/mol
Carbon dioxide	CO_2	2.370	0.817	44
Nitrogen	N_2	0.310	0.809	28
Methane	C_1	73.190	0.300	16
Ethane	C_2	7.800	0.356	30
Propane	C_3	3.550	0.507	44
iso-Butane	i-C_4	0.710	0.563	58
n-Butane	n-C_4	1.450	0.584	58
iso-Pentane	i-C_5	0.640	0.624	72
n-Pentane	n-C_5	0.680	0.631	72
Hexanes	SCN6	1.090	0.685	84
SCN7 to SCN9	MCN1	3.247	0.747	106
SCN10 to SCN13	MCN2	2.141	0.797	151
SCN14 to SCN17	MCN3	1.142	0.838	211
SCN18 to SCN24	MCN4	0.975	0.869	282
C_{25+}	MCN5	0.705	0.919	462

2.4 Tuning of the Peng-Robinson (1976) EOS after Lumping

The tuning technique of Hosein and Dawe (2011) with the Peng-Robinson (1976) EOS as stated earlier was re-applied, using the lumped compositions in Table 2. BIC (Soave 1972; Oellrich et al 1981) between methane and the MCN groups, Ω_a and Ω_b for methane and Ω_a and Ω_b for the last MCN group (MCN5) are difficult to determine parameters as discussed by Hosein and Dawe (2011) and were selected as the main tuning parameters. The parameters of Ω_a and Ω_b for the other MCN groups (MCN1 to MCN4) were selected for minor tuning (WINPROP

2002). The selected parameters were adjusted as a group (Agarwal et. al. 1990) so as to reduce the objective function F to a minimum (Dennis et. al., 1981) as shown earlier in Eq. 3. The predicted physical property data after lumping are given in Tables 3, 6 and 7.

3. RESULTS AND DISCUSSION

The experimental and tuned EOS (Peng-Robinson 1976) predicted data before and after lumping are presented in Tables 3 to 7. The differences between the predicted and experimental data before and

$$\text{Difference (Diff. in \%)} = \frac{[\text{y pred.} - \text{y expt.}]}{\text{y expt.}} \times 100 \quad (4)$$

after lumping for both samples A and B is less than ±1.0 % for dew point pressure (Table 3), less than ±3.0 % for gas compressibility factor, less than ±8.0 % for liquid volume and less than ±5.0 % for produced gas (Tables 4 to 7). The differences between the tuned EOS (Peng-Robinson 1976) predicted data before and after lumping is generally less than ±1.0 % for dew point pressure, gas compressibility factor and produced gas and less than ±4.0 % for liquid volume as shown in Table 8. These results indicate that the Whitson's (1980) lumping scheme when applied with Hosein and Dawe (2011) tuning technique can give accurate, and similar, predictions to those obtained before lumping.

Table 3
Differences (Diff. in %) between Predicted (Pred.) and Experimental (Expt.) Dew Point Pressure (DPP) for Trinidad Sample A and North Sea Sample B, before and after Lumping

Sample	Before Lumping			After Lumping	
	Expt. DPP	Pred. DPP	Diff. in	Pred. DPP	Diff. in
	psia	psia	%	psia	%
Sample A	5159.7	5144.0	-0.30	5142.0	-0.34
Sample B	6764.7	6744	-0.31	6744	-0.31

Table 4
Differences (Diff. in %) between Peng-Robinson (1976) EOS Predicted (Pred.) and Experimental (Expt.) Gas Compressibility (Z) Factor, Liquid Volume (LDO) and Produced Gas (PG) after tuning with Composition to SCN24 for Trinidad Sample A (No Lumping)

Pressure,	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in
psia	Z Factor	Z Factor	%	LDO, %	LDO, %	%	PG, %	PG, %	%
5159.7	0.000	0.000	0.00	0.0	0.0	0.00	0.0	0.0	0.00
4414.7	0.957	0.970	1.36	1.3	1.2	-7.69	9.7	10.0	3.09
3614.7	0.918	0.926	0.87	2.5	2.6	4.00	22.5	22.9	1.76
2814.7	0.902	0.900	-0.22	3.5	3.7	5.71	37.9	38.1	0.52
2014.7	0.908	0.896	-1.32	4.0	4.1	2.50	55.3	55.0	-0.45
1314.7	0.928	0.912	-1.72	4.0	4.1	2.50	71.0	70.7	-0.39
714.7	0.956	0.942	-1.46	3.8	3.9	2.63	84.2	83.9	-0.31

Table 5
Differences (Diff. in %) between Peng-Robinson (1976) EOS Predicted (Pred.) and Experimental (Expt.) Gas Compressibility (Z) Factor, Liquid Volume (LDO) and Produced Gas PG) after tuning with Composition to SCN24 for North Sea Sample B (No Lumping)

Pressure,	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in
psia	Z Factor	Z Factor	%	LDO, %	LDO, %	%	PG, %	PG, %	%
6764.7	0.000	0.000	0.00	0.00	0.0	0.00	0.0	0.0	0.00
5514.7	1.089	1.095	0.55	14.1	13.0	-7.80	9.0	9.4	4.17
4314.7	0.972	0.980	0.82	19.7	19.8	0.51	21.7	21.9	0.72
3114.7	0.913	0.915	0.22	21.6	22.7	5.09	38.7	38.6	-0.19
2114.7	0.914	0.901	-1.42	21.3	22.2	4.23	55.7	55.6	-0.15
1214.7	0.937	0.917	-2.13	20.2	20.6	1.98	72.1	72.3	0.21
714.7	0.960	0.939	-2.19	19.3	19.4	0.52	81.3	81.8	0.61

Table 6
Differences (Diff. in %) between Peng-Robinson (1976) EOS Predicted (Pred.) and Experimental (Expt.) Gas Compressibility (Z) Factor, Liquid Volume (LDO) and Produced Gas (PG) for Trinidad Sample A, after Lumping and Tuning

Pressure,	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in
psia	Z Factor	Z Factor	%	LDO, %	LDO, %	%	PG, %	PG, %	%
5159.7	0.000	0.000	0.00	0.0	0.0	0.00	0.0	0.0	0.00
4414.7	0.957	0.970	1.36	1.3	1.2	-7.69	9.7	10.0	3.09
3614.7	0.918	0.926	0.83	2.5	2.5	0.00	22.5	22.9	1.76
2814.7	0.902	0.899	-0.33	3.5	3.6	2.86	37.9	38.1	0.52
2014.7	0.908	0.895	-1.43	4.0	4.1	2.50	55.3	55.0	-0.45
1314.7	0.928	0.912	-1.72	4.0	4.1	2.50	71.0	70.7	-0.39
714.7	0.956	0.942	-1.46	3.8	3.8	0.00	84.2	84.0	-0.19

Table 7
Differences (Diff. in %) between Peng-Robinson (1976) EOS Predicted (Pred.) and Experimental (Expt.) Gas Compressibility (Z) Factor, Liquid Volume (LDO) and Produced Gas (PG) for North Sea Sample B, after Lumping and Tuning

Pressure,	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in	Expt.	Pred.	Diff. in
psia	Z Factor	Z Factor	%	LDO, %	LDO, %	%	PG, %	PG, %	%
6764.7	0.000	0.000	0.00	0.00	0.0	0.00	0.0	0.0	0.00
5514.7	1.089	1.095	0.55	14.1	13.0	-7.80	9.0	9.4	4.17
4314.7	0.972	0.980	0.82	19.7	19.8	0.51	21.7	21.9	0.72
3114.7	0.913	0.915	0.22	21.6	22.8	5.56	38.7	38.6	-0.19
2114.7	0.914	0.901	-1.42	21.3	22.3	4.69	55.7	55.5	-0.33
1214.7	0.937	0.917	-2.13	20.2	20.6	1.98	72.1	72.3	0.21
714.7	0.960	0.939	-2.19	19.3	19.4	0.52	81.3	81.8	0.61

Table 8
Calculated Differences (Diff. in %) in the Predicted Dew Point Pressure (DPP), Gas Compressibility (Z) Factor, Liquid Volume (LDO) and Produced Gas (PG) before and after Lumping, for Trinidad Sample A (Tables 3, 4 and 6) and for North Sea Sample B (Tables 3, 5 and 7)

Trinidad Sample A				North Sea Sample B			
Diff. in %	Diff. in %	Diff. in %	Diff. in %	Diff. in %	Diff. in %	Diff. in %	Diff. in %
DPP	Z Factor	LDO	PG	DPP	Z Factor	LDO	PG
-0.039	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	0.00	0.00		0.00	0.00	0.00
	-0.04	-3.85	0.00		0.00	0.00	0.00
	-0.11	-2.70	0.00		0.00	0.44	0.00
	-0.11	0.00	0.00		0.00	0.45	-0.18
	0.00	0.00	0.00		0.00	0.00	0.00
	0.00	-2.56	0.12		0.00	0.00	0.00

CONCLUSIONS

1. With Whitson's (1980) lumping scheme accurate predictions of dew point pressure, gas compressibility factor, liquid volume and produced gas were obtained for a lean and a rich gas condensate samples when the Peng-Robinson (1976) EOS was tuned with BIC and the Ω's.

2. The accuracy obtained with Whitson's (1980) lumping scheme show that it can be applied in compositional simulation studies and complex forms of lumping and algorithms to select the best lumping schemes are not required.

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APPENDIX

Example Calculation using Whitson's (1980) Lumping Scheme with Sample A (Table 1)

Step 1: The numbers of MCN groups, N_g = Integer [1 + 3.3 Log (N – n)] A1

where n is the number of carbon atoms of the first heavy SCN group (SCN7) and N is number of carbon atoms of the plus (last) fraction (C_{25+}). From Table 1, n = 7 and N = 25. By substituting for n and N in Eq. A1, the numbers of MCN groups, Ng = Integer [1 + 3.3 Log (25 – 7)] = 5.

Step 2: The distribution of SCN groups within each MCN group are determined from molecular weight boundaries as follows: $(M)_I = (M)_n$ [Exp. $\{(1 / N_g)$ Ln. $((M)_N / (M)_n)\}]^I$ A2

Where $(M)_n$ is the molecular weight of the first heavy SCN group (SCN7), $(M)_N$ is the molecular weight of the plus (last) fraction (C_{25+}) and I =1, 2, ….., N_g,. From Table 1 $(M)_n$ = 96 and $(M)_N$ = 398. By substituting for $(M)_n$, $(M)_N$ and N_g in Eq. A2, the molecular weight boundaries and distribution of SCN groups in each MCN group were determined as follows:

$(M)_1 = 96$ [Exp. $\{(1 / 5)$ Ln. $(398 / 96)\}]^1 = 128$. The MCN1 group is from SCN7 to SCN9

$(M)_2 = 96$ [Exp. $\{(1 / 5)$ Ln. $(398 / 96)\}]^2 = 170$. The MCN2 group is from SCN10 to SCN12

$(M)_3 = 96$ [Exp. $\{(1 / 5)$ Ln. $(398 / 96)\}]^3 = 225$. The MCN3 group is from SCN13 to SCN16

$(M)_4 = 96$ [Exp. $\{(1 / 5)$ Ln. $(398 / 96)\}]^4 = 299$. The MCN4 group is from SCN17 to SCN21

$(M)_5 = 96$ [Exp. $\{(1 / 5)$ Ln. $(398 / 96)\}]^5 = 398$. The MCN5 group is from SCN22 to C_{25+}

The above two calculation steps were repeated for sample B and the results obtained for both samples were presented in Table 2. The distribution of SCN groups in each MCN group was determined from Table 1 by selecting the SCN groups whose molecular weights are within the boundaries of the molecular weights calculated above.

