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A Consistent Procedure for the Estimation of Pseudo-Component Properties

C.F. Leibovici, P.L. Govel, and Thomas Piacentino, Elf Aquitaine Production

SPE Members

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ABSTRACT

A new method is presented for the estimation of physical properties of pseudo-components generated by any lumping procedure. Completely consistent with the equation of state to be used for the description of the thermodynamic behaviour of the lumped system, this method tends to minimize the loss of information induced by component lumping. Applied to complex fluids, it has been proved to be very effective. For illustration purposes, some results are reported for a North Sea gas condensate and a Gulf of Guinea light oil.

INTRODUCTION

When a reservoir fluid is characterized on the basis of several hundreds of identified components plus many heavy fractions more or less accurately defined, the first typical task to achieve is a substantial lumping of the system in order to reduce the size of further thermodynamic computations. Typically, fundamental studies and process simulations handle 15-30 components and fractions while reservoir compositional simulations are generally limited to significantly less pseudo-components.

It is obvious that grouping so many components together results in lost information and flexibility. Reduced flexibility is unavoidable but can be limited through an optimal clustering scheme as proposed by Montel and Gouel¹ and lost information may be minimized using proper techniques.

The goal of this paper is to show that a new simple approach, totally based on the equation of state to be used latter, can overcome most of the problem through a more consistent evaluation of both properties associated to lumped systems and interaction parameters between pairs of these groups.

PROPOSED METHOD

When thermodynamic calculations are based on equations of state, pure component parameters are needed; in the most general case, they are derived from standard physical properties (critical temperature and pressure, acentric factor, molecular weight, ...). In this paper, it will be assumed that, for any component, all requested physical properties are available.

Up to now, it seems that, once the lumping scheme has been decided, the problem has been systematically set in the following manner : knowing the molar composition of the components in a given group and the properties of the individuals belonging to the group, what is the value to assign to each property for the group ? Such an approach leads to more or less simple methods consisting basically on an appropriate weighting of properties or combination of properties.

The simplest method consists in the use of Kay's rule² which just assumes that any property can be expressed as a linear combination of component properties, weighting factors corresponding to mole fractions.

$$T_{cm} = \sum_{i=1}^N x_i \cdot T_{ci} \quad P_{cm} = \sum_{i=1}^N x_i \cdot P_{ci} \quad \omega_m = \sum_{i=1}^N x_i \cdot \omega_i \quad (1)$$

More sophisticated methods, using the equation of state itself, have been proposed for estimating the physical properties of the group; they basically use the mixing rules formulation for parameter identification. In the case of cubic equations of state

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + u b V + w b^2} \quad (2)$$

and classical Van der Waals mixing rules,

$$a_m = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \sqrt{a_i \cdot a_j} \cdot (1 - k_{ij}) \quad (3a)$$

$$b_m = \sum_{i=1}^N x_i \cdot b_i \quad (3b)$$

the pseudo-critical parameters looked for can be easily identified³.

The method which is proposed here is based on a rigorous identification of the equation of state parameters computed at various temperatures for both the detailed mixture and the lumped system. Once this parameter identification has been performed, more traditional properties [eg: T_c , P_c , ω] can be eventually derived from the lumped equation of state parameters. This approach, which will be illustrated here in the limited frame of classical cubic equations of state and mixing rules, can easily be applied to any other situations even if leading to more complex and/or less explicit formulations.

Critical temperature and critical pressure

Assuming that u and w are component independent^{4,5} and that the a parameter is temperature dependent [$a = a_c f(T)$], the pseudo critical temperature T_{cm} and pressure P_{cm} are [whatever the generic parameters u and w could be] solutions of the following set of non linear equations

$$\frac{T_{cm}^2}{P_{cm}} = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \frac{T_{ci} \cdot T_{cj}}{\sqrt{P_{ci} \cdot P_{cj}}} \cdot \sqrt{f_i(T_{cm}) \cdot f_j(T_{cm})} \cdot (1 - k_{ij}) \quad (4a)$$

$$\frac{T_{cm}}{P_{cm}} = \sum_{i=1}^N x_i \cdot \frac{T_{ci}}{P_{ci}} \quad (4b)$$

which easily reduces, by elimination of P_{cm} , to one equation and one unknown T_{cm} . Depending on the analytical expression of temperature functions, the equation to solve will be more or less complex but will not present any major difficulty; in the most popular case where $f(T)$ is a perfect square of a linear expression with respect to \sqrt{T} ^{4,5}, T_{cm} is just solution of a quadratic equation in $\sqrt{T_{cm}}$.

Very often, the equations which are solved ignore the temperature dependences on the right hand side of equation (4a) and just reduce to the evaluation of T_{cm} and P_{cm} according to equations (5a) and (5b)

$$\frac{T_{cm}^2}{P_{cm}} = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \frac{T_{ci} \cdot T_{cj}}{\sqrt{P_{ci} \cdot P_{cj}}} \cdot (1 - k_{ij}) \quad (5a)$$

$$\frac{T_{cm}}{P_{cm}} = \sum_{i=1}^N x_i \cdot \frac{T_{ci}}{P_{ci}} \quad (5b)$$

In that case, the acentric factor of the lumped system is obtained using Kay's rule¹

$$\omega_m = \sum_{i=1}^N x_i \cdot \omega_i \quad (5c)$$

Temperature dependence

In the procedure proposed here, the exact solution of equations (4a) and (4b) is just the first step. Both T_{cm} and P_{cm} parameters being now available, the process will continue by the identification of temperature dependences for the lumped system. This identification will consist in finding the numerical values of the $f_m(T)$ function which, for any temperature lower than T_{cm} , satisfies equation (6)

$$\frac{T_{cm}^2}{P_{cm}} \cdot f_m(T) = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \frac{T_{ci} \cdot T_{cj}}{\sqrt{P_{ci} \cdot P_{cj}}} \cdot \sqrt{f_i(T) \cdot f_j(T)} \cdot (1 - k_{ij}) \quad (6)$$

This presents a very strong analogy with what is usually done when adjusting the value of the $f_i(T)$ function on vapor pressure data points for a pure component.

Once the function $f_m(T)$ has been tabulated for a series of temperature values (we use 50 equispaced points ranging between 0.5 T_{cm} and T_{cm}), the parameters appearing in its analytical expression can be easily identified via any classical least squares fit procedure. From there, if needed for any other purposes, the acentric factor of the lumped system can be derived by a search of the vapor pressure of this pseudo component at 0.7 T_{cm} .

Unlike other approaches, this procedure ensures that, over a wide range of temperature, the equation of state parameters associated to the initial and the lumped systems will be almost identical.

Binary interaction parameters between pseudo-components

The same procedure can also be used to generate consistent interaction parameters between lumped groups. For simplicity, we shall assume that the N component mixture has to be lumped in two pseudo-components A and B . In such a case, the parameters for A and B will be first obtained solving equations (7a) and (7b) for T_{cmA} , P_{cmA} , T_{cmB} , P_{cmB}

$$x_K^2 \cdot \frac{T_{cmK}^2}{P_{cmK}} = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \frac{T_{ci} \cdot T_{cj}}{\sqrt{P_{ci} \cdot P_{cj}}} \cdot \sqrt{f_i(T_{cmK}) \cdot f_j(T_{cmK})} \cdot (1 - k_{ij}) \cdot \delta_{iK} \cdot \delta_{jK} \quad (7a)$$

$$x_K \cdot \frac{T_{cmK}}{P_{cmK}} = \sum_{i=1}^N x_i \cdot \frac{T_{ci}}{P_{ci}} \cdot \delta_{iK} \quad (7b)$$

K being either A or B and

$$x_K = \sum_{i=1}^N x_i \cdot \delta_{iK}$$

δ_{iK} being 1 if component i belongs to group K and 0 otherwise. In a second step, discrete values of the function $f_{mK}(T)$ are generated using equation (8)

$$x_K^2 \cdot \frac{T_{cmK}^2}{P_{cmK}} \cdot f_{mK}(T) = \sum_{i=1}^N \sum_{j=1}^N x_i \cdot x_j \cdot \frac{T_{ci} \cdot T_{cj}}{\sqrt{P_{ci} \cdot P_{cj}}} \cdot \sqrt{f_i(T) \cdot f_j(T)} \cdot (1 - k_{ij}) \cdot \delta_{iK} \cdot \delta_{jK} \quad (8)$$

and curve-fitted to any desired analytical expression. Once these parameters have been obtained for A and B , it is possible to mix these two pseudo-components and request again that the pseudo-critical point of this binary be identical to the pseudo-critical point of the original mixture. Since, at this level, all requested parameters are known, the interaction parameters k_{AB} are immediately obtained applying equations (4a) to the overall mixture and the (A+B) binary. This is only needed if there is at least one non-zero k_{ij} [i belonging to A and j to B] since the effects of non-zero k_{ij} inside the same pseudo-component have been already taken into account during the evaluation of critical temperature, critical pressure and temperature dependences.

It is obvious that the generalization of such an approach to any number of pseudo-components does not present any problem.

APPLICATION TO A SIMPLE CASE

In order to illustrate the proposed method, an equimolar mixture of methane, ethane, propane, n-butane, n-pentane and n-hexane has been considered. All needed physical properties were retrieved from the DIPPR data bank and the standard form of the Peng-Robinson⁵ equation of state was used without any binary interaction parameter.

For this wide boiling mixture [at atmospheric pressure, the difference between dew and bubble temperatures is 166 K], the PT line corresponding to a vapor fraction of 0.5 has been computed in order to simulate a molar average boiling point (MABP) curve [for this mixture, the true critical point coordinates are 428.62 K and 6.7138 MPa]. Then, the total mixture has been lumped in one pseudo-component the properties of which being computed according to either

- Case 1 : equation (1)
- Case 2 : equations (5a), (5b) and (5c)
- Case 3 : equations (4a), (4b), (6)

The properties obtained according to the different procedures are summarized in Table 1. They do not reveal major differences for any of the parameters. But, in a second step, for each of these three cases, the vapor pressure curve of the generated pseudo-component has been computed on the basis of the same equation of state. The results, summarized in Table 2, have to be compared to the corresponding MABP curve points computed for the original mixture.

Now, very large differences appear since :

- cases 1 and 2 systematically overestimates the vapor pressure by 20 to 50 %

- case 3 gives always a vapor pressure more reasonably closer to the MABP curve

This improvement is significant since, when tuning equation of state parameters, only properties associated to the end fractions are usually modified. But, if light components - eg : all C_6 , C_7 and C_8 components - are lumped together and the vapor pressure of the generated pseudo-component does not reflect adequately the volatility of the original system, then it will be left to heavy fractions parameters to correct for this inconsistency. Obviously, this is not the role of these parameters in PVT data matching !

APPLICATION TO RESERVOIR FLUIDS

The proposed method has been applied to a gas condensate from the North Sea and a light oil from the Gulf of Guinea. In both cases, the initial detailed experimental analysis [161 and 173 components plus fractions] was first used to generate 27 components and pseudo-components. The component properties and mole percents are reported in tables 3 and 4. The properties of the last two fractions were adjusted in order to match as well as possible all experimental data available from Elf Aquitaine Production PVT laboratory.

In a second step, the first 25 pseudo-components were lumped into 8 and then 3 clusters in order to generate 10 and 5 pseudo-component systems to be used in reservoir simulations; this was done using the dynamic clustering method proposed earlier by Montel and Gouel¹.

The enclosed figures, which resume the comparison of results obtained for the detailed and lumped fluids, are just briefly commented :

Gas condensate

- the phase envelope, which exhibit an unusual behaviour [confirmed by saturation pressure measurements], are identical.
- the gas compressibility factor curves overlap almost perfectly.
- the liquid dropout curves differ slightly when the number of pseudo-components is reduced down to 5. This is mainly due to changes in the liquid density computed from the same equation of state. The differences are significantly smaller if the liquid density is computed by a method other than the equation of state itself.

Light oil

- the three curves (phase envelopes, oil FVF and dissolved gas) are identical for 10 and 27 pseudo-components. When the number of these is reduced to 5, the curves are slightly shifted.

Remarks

- When the number of pseudo-components is reduced to 5, the shift of the curves can easily be reduced by small changes of the physical properties of the last two fractions.
- This level of agreement between results obtained for 27, 10 or 5 components was unreachable in the frame of Kay's or classical formulations.

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APPENDICES**Table 1 : Properties of the lumped system**

Physical property	Case 1	Case 2	Case 3
Critical Temperature (K)	378.01	375.36	391.05
Critical Pressure (MPa)	3.985	3.687	3.841
Acentric Factor	0.1694	0.1694	0.1784

Table 2 : Vapor pressure of the lumped system

T (K)	M A B P (MPa)	Case 1	Case 2	Case 3
260	0.1413	0.2293	0.2262	0.1568
270	0.2038	0.3220	0.3168	0.2239
280	0.2856	0.4407	0.4326	0.3111
290	0.3905	0.5897	0.5776	0.4220
300	0.5224	0.7735	0.7562	0.5603
310	0.6852	0.9970	0.9729	0.7302
320	0.8834	1.2650	1.2325	0.9357
330	1.1215	1.5828	1.5399	1.1814
340	1.4040	1.9558	1.9005	1.4717
350	1.7360	2.3900	2.3196	1.8117
360	2.1225	2.8913	2.8034	2.2063
370	2.5690	3.4664	3.3579	2.6611
380	3.0811	-	-	3.1817
390	3.6646	-	-	3.7743
400	4.3261	-	-	-

Table 3 : Gas condensate characterization

	T_c (K)	P_c (MPa)	ω	Mw	% mole
N2	126.20	3.394	0.0400	28.01	0.3243
CO2	304.20	7.377	0.2250	44.01	1.9549
C1	190.60	4.600	0.0115	16.04	76.1530
C2	305.40	4.884	0.0908	30.07	7.7367
C3	369.80	4.245	0.1454	44.10	3.6177
iC4	408.10	3.648	0.1760	58.12	0.5667
nC4	425.20	3.800	0.1928	58.12	1.3258
iC5	460.26	3.383	0.2271	72.15	0.4480
nC5	469.60	3.374	0.2273	72.15	0.6100
CC5	511.60	4.509	0.1923	70.14	0.0580
PC6	503.79	3.007	0.2860	86.18	0.6001
CC6	547.41	3.990	0.2215	84.16	0.4148
AC6	562.10	4.894	0.2100	78.11	0.1735
PC7	536.44	2.760	0.3364	100.21	0.4239
CC7	566.27	3.469	0.2451	98.19	0.5056
AC7	591.70	4.114	0.2566	92.14	0.3063
PC8	565.05	2.502	0.3816	114.23	0.3291
CC8	594.05	2.974	0.2391	112.21	0.2540
AC8	619.46	3.584	0.3228	106.16	0.2564
PC9	590.64	2.329	0.4230	128.25	0.2630
CC9	621.21	2.839	0.2998	125.97	0.1640
AC9	644.06	3.208	0.3725	120.16	0.1217
PC10	613.72	2.146	0.4646	142.28	0.2411
CC10	621.58	2.625	0.4058	140.20	0.0427
AC10	670.83	2.972	0.3642	133.80	0.1049
CN-1	711.04	1.875	0.8000	240.00	2.6703
CN-2	848.08	1.633	1.3000	450.26	0.3338

Table 4 : Light oil characterization

	T_c (K)	P_c (MPa)	ω	Mw	% mole
N2	126.20	3.394	0.0400	28.01	0.3706
CO2	304.20	7.377	0.2250	44.01	0.7512
C1	190.60	4.600	0.0115	16.04	56.3090
C2	305.40	4.884	0.0908	30.07	10.0070
C3	369.80	4.245	0.1454	44.10	4.8672
iC4	408.10	3.648	0.1760	58.12	0.8245
nC4	425.20	3.800	0.1928	58.12	1.6569
iC5	460.40	3.384	0.2273	72.15	0.8065
nC5	469.60	3.374	0.2273	72.15	1.0908
CC5	511.60	4.509	0.1923	70.14	0.0886
PC6	503.86	3.005	0.2862	86.18	1.5758
CC6	543.01	3.930	0.2268	84.16	0.4710
AC6	562.10	4.894	0.2100	78.11	0.1304
PC7	537.08	2.758	0.3386	100.21	1.1471
CC7	563.31	3.468	0.2495	98.19	0.7720
AC7	591.70	4.114	0.2566	92.14	0.3130
PC8	564.91	2.502	0.3816	114.23	0.9544
CC8	591.21	2.952	0.2363	112.21	0.6199
AC8	619.24	3.577	0.3245	106.16	0.4664
PC9	590.89	2.330	0.4238	128.25	0.8060
CC9	625.53	2.807	0.2948	126.23	0.4545
AC9	645.41	3.220	0.3820	120.16	0.3364
PC10	611.73	2.142	0.4621	142.28	0.7381
CC10	664.24	2.943	0.2718	140.15	0.1697
AC10	674.87	3.058	0.3841	133.21	0.3481
CN-1	683.15	2.399	0.6121	191.74	8.7415
CN-2	838.15	1.285	0.6799	387.42	5.1828

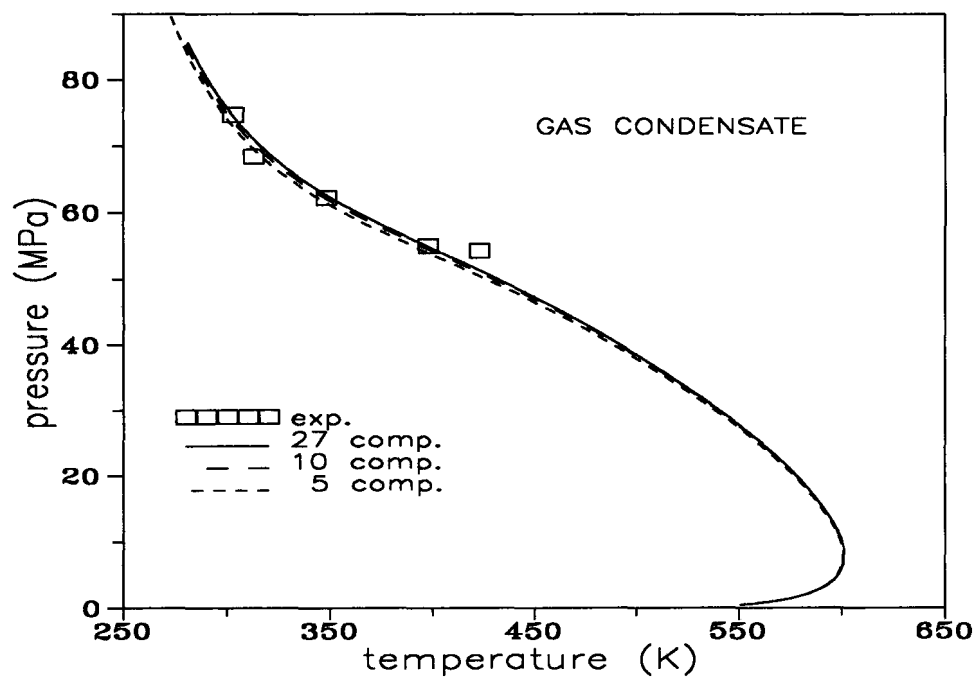


Fig. 1 : Phase envelope

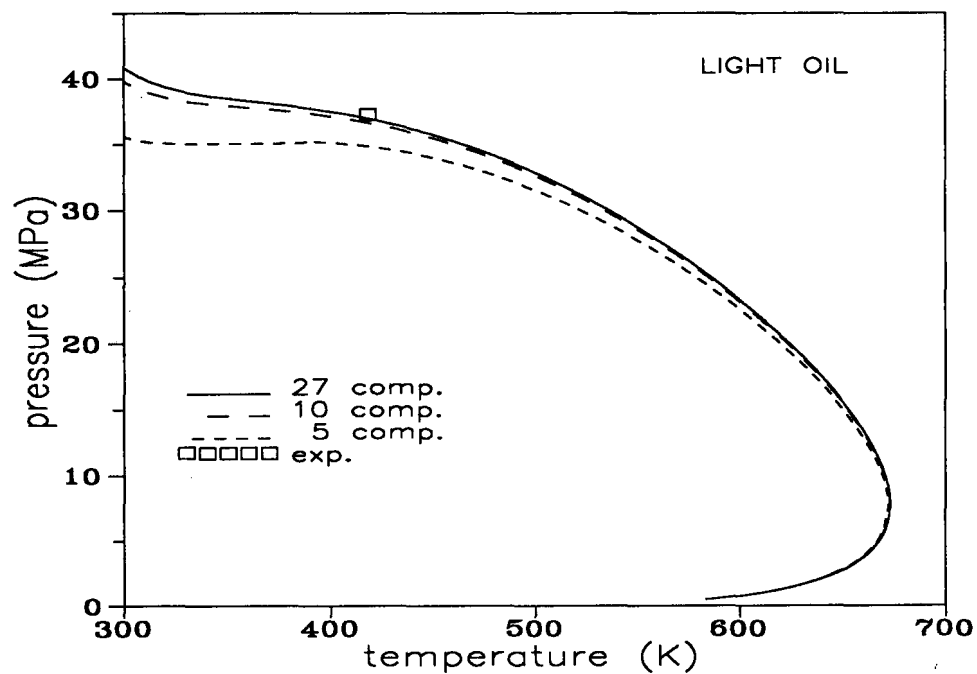


Fig. 2 : Phase envelope

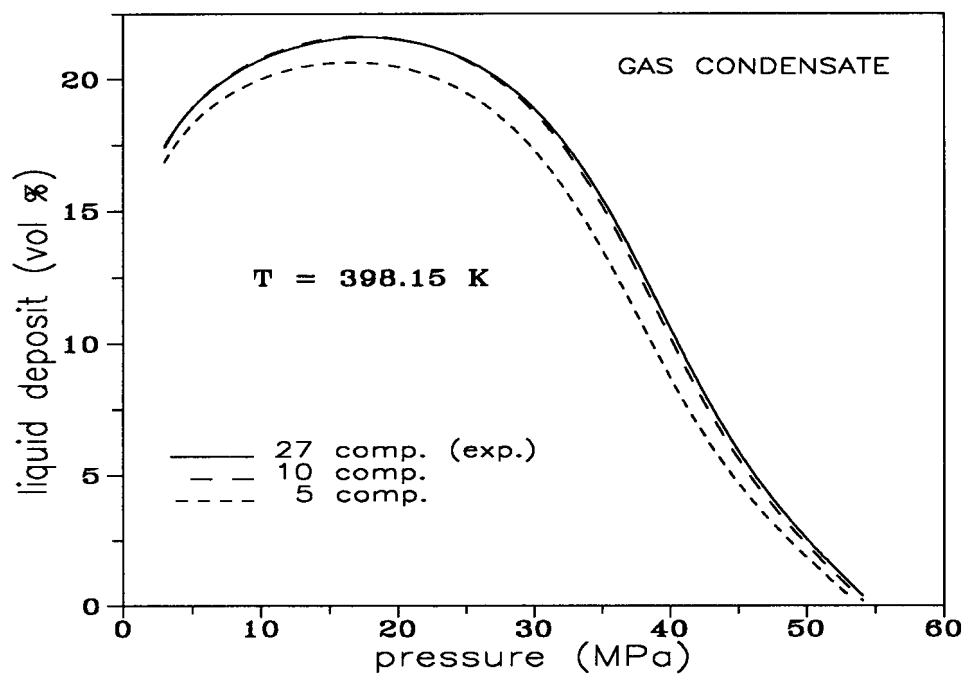


Fig. 3 : Liquid deposit

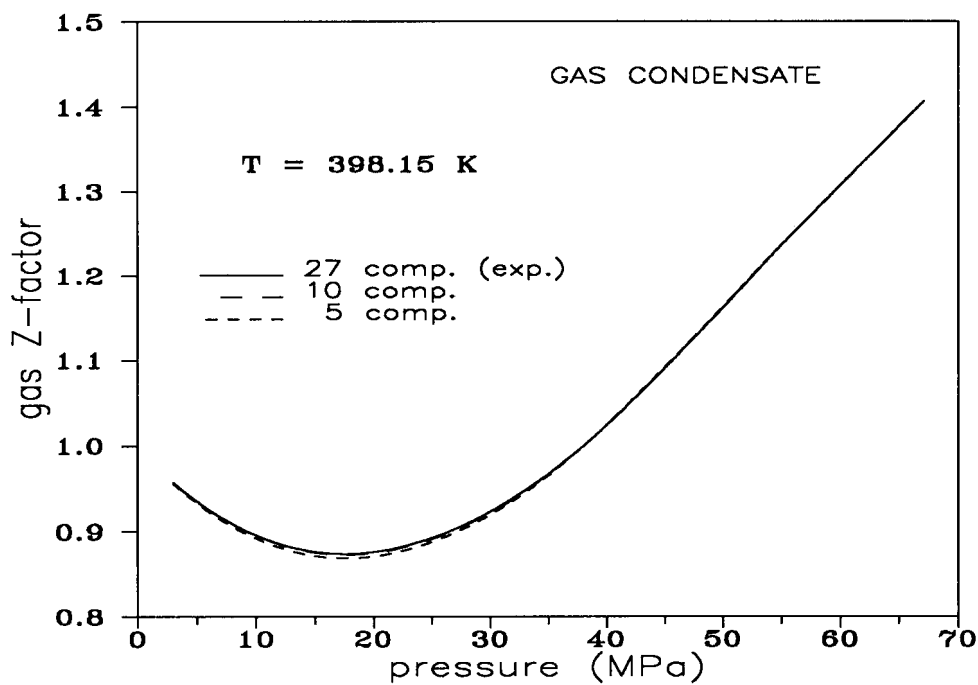


Fig. 4 : Gas compressibility factor

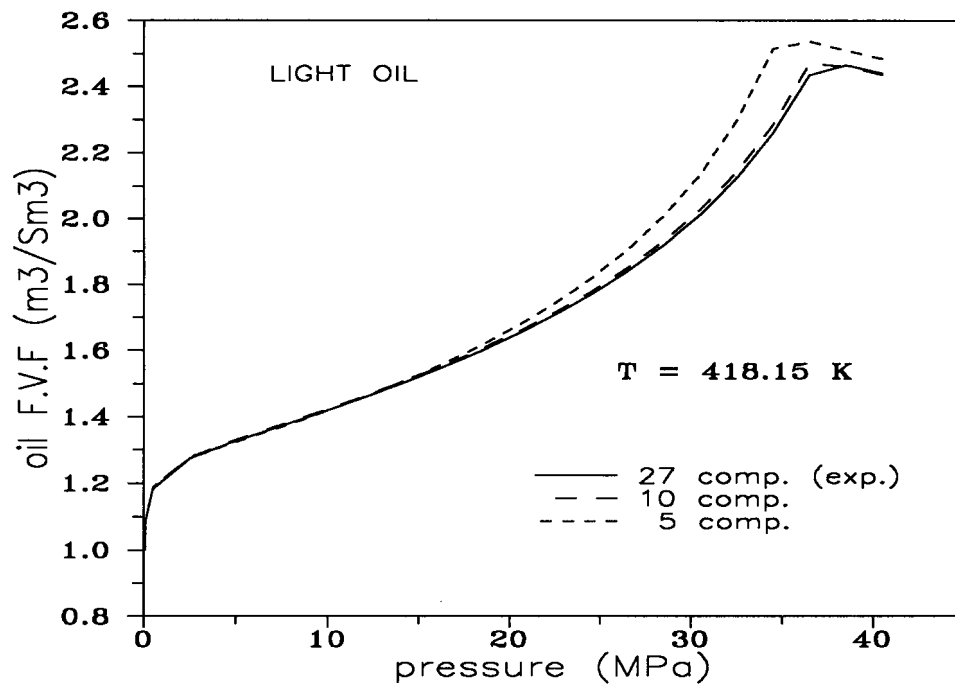


Fig. 5 : Oil F.V.F vs pressure

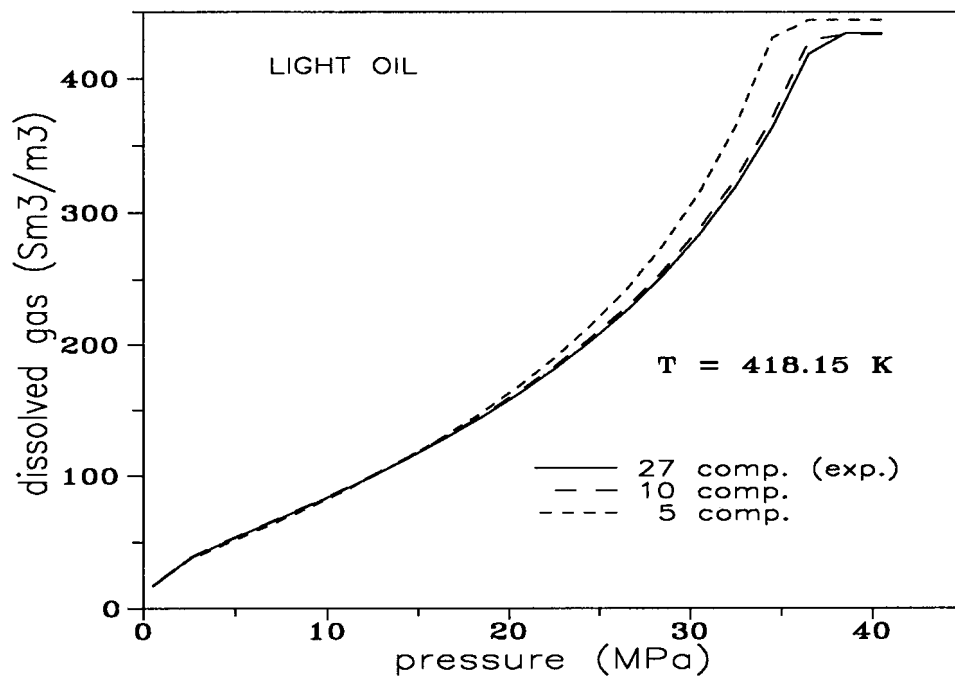


Fig. 6 : Rs vs pressure