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# Risks of empirical correlations for pseudo-critical properties of natural gas

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#### Abstract

There are given estimates of the influence of uncertainties when using empirical correlations for pseudocritical characteristics of natural gas with its density on the results of estimates of gas reserves and bottomhole pressures.

Modeling on the examples of the calculation of the blowout pressure in a gas well and the creation of a material balance of a gas deposit showed that their influence on the overall modeling error can be comparable to the contribution of instrumental errors only with high-precision measurements of pressure and temperature. When determining the gas supercompressibility coefficient based on the pseudocritical gas characteristics, about 70 % of the errors will be associated with the variation in the calculation of the pseudocritical temperature

Keywords: acentric factor, compressibility factor, material balance, Monte Carlo method.

The modern scientific paradigm assumes that when calculating the properties of natural gas under different thermobaric conditions, there are used the equation of state and the principle of corresponding states, which in turn assumes knowledge of the pseudocritical characteristics of the gas. In the oil and gas industry, such calculations are made, for example, when creating models of the material balance of gas deposits and well testing in order to calculate the current reservoir pressure in the deposit.

Creating a material balance of gas deposits is a simple and effective tool for analyzing the development of a field and assessing the average indicators of individual deposits, in particular, the initial gas reserves and the initial reservoir pressure in the deposit, the activity of the aquifer. The complete closed system of equations underlying the creation of the reservoir material balance model and the principles of its adaptation to the real history of the field development were formulated by us in [1].

In practice, to estimate gas reserves in a reservoir, a simplified material balance model for a closed gas reservoir is often used, when there is no external water inflow, the pore gas-saturated volume does not change, and the reservoir temperature is constant. This model results in a linear relationship between the reduced reservoir pressure p/z and the recoverable gas volume  $V_{prod.t.}$ . This dependence is used both in the gas drive recovery mechanism and with insignificant activity of the aquifer, neglecting the resulting errors.

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 2022, Ivano-Frankivsk National Technical University of Oil and Gas. All rights reserved. In the future, the accuracy of estimating gas reserves in a deposit determines, first of all, the reliability of forecasting the dynamics of gas production and the adequacy of the adopted technological solutions to improve the development system for individual deposits and the gas field as a whole.

When using a simplified material balance model, the accuracy of the result will depend on the accuracy of determining the cumulative gas production, reservoir pressure and the corresponding value of the gas compressibility factor.

The accuracy of measuring cumulative gas production is related to the instruments used. They, as a rule, have an accuracy class of at least 1 %.

Reservoir pressure in wells is determined by direct measurement with a depth gauge and more often by recalculating the pressure measured at the wellhead from a shut-in well to bottomhole conditions. The accuracy of pressure measurement with modern depth gauges is high; it is not lower than 0.03 % of the results in general. When measuring wellhead pressure, as a rule, pressure gauges with an accuracy class of at least 1 % are used, and conversion to bottomhole conditions is carried out according to the barometric formula, which also gives a certain error.

The material balance equation involves the recalculation of gas volumes from reservoir conditions to surface conditions using the gas supercompressibility factor and the principle of corresponding states. It is believed that the gas supercompressibility factor can be reliably determined by the Soave–Redlich–Kwong equation [2], the coefficients of which are calculated using the pseudocritical pressure (pseudocritical pressure)  $p_{pc}$ , pseudocritical temperature  $T_{pc}$  and the acentric factor.



Figure 1 – Correlation for pseudocritical pressure

New correlations for gas fields in the Dnieper-Donets depression

In practice, for natural gas of a certain composition, given their close correlation with the relative density  $\gamma$  of the gas relative to air, they are calculated using empirical regression equations. More often they refer to Standing [3]. Sutton correlation [4, 5], based on the data of laboratory experiments, which gives refined regression dependences separately for associated gases and gas condensate mixtures. Elsharkawy and Elkamel [6] offer their own correlations obtained for gases with a wider density range. OAO "Gazprom" instruction issued in 1980 [7] for simplified calculations recommends regression dependencies for pseudocritical pressure and temperature on the molar mass M of the gas.

For practical use, correlations for heavy components are also important. The Two [8], Lee– Kesler [9], Cavett [10], and Riasi et al. correlations [10, 11] are often referred to, presented in several versions as dependences of pseudocritical pressure and temperature on the density and boiling point of hydrocarbons.

The most significant non-hydrocarbon gas components are nitrogen, helium, carbon dioxide and hydrogen sulfide. It is believed [12, 13] that their content of more than 5 % has a significant impact on the accuracy of calculating gas parameters. At high concentrations of these components, the error in determining the supercompressibility factor can exceed 10 %.

To take into account the special effect of acidic components, many authors consider it possible to use the correction proposed by Wichert and Aziz to the pseudocritical characteristics calculated for the hydrocarbon component of the gas [4, 6, 7 and others]. Moreover, the proposed formulas for calculating the correction give similar results [14].

Based on the results of 150 gas condensate studies of the production of wells in the Dnieper-Donets depression, we [12] built a correlation of pseudocritical pressure, pseudocritical temperature and acentricity factor with the density relative to air of only the hydrocarbon component of reservoir gases. The fields of the Dnieper-Donets depression are characterized by a wide range of reservoir pressures and temperatures, the composition of gases varies from dry to wet with a relatively low content of non-hydrocarbon components. Figures 1–3 illustrate the tight relationship between the actual pseudo-critical values of pressure and temperature and the acentricity factor for the hydrocarbon component of natural gas, calculated from the results of laboratory studies of reservoir gases composition of the Dnieper-Donets basin fields with its relative density.

If for the critical temperature all correlations are close to the actual data, then for the critical pressure the best of them – the Standing correlation for "dry" gases and the Gazprom Instructions for "wet" gases with a relatively higher density – differ noticeably from the experimental data.

According to the data of natural gases from the fields of the Dnipro-Donets depression with estimates of the confidence intervals of the regression parameters by the value of the residual variance with a confidence level of 95 %, they are as follows:



Figure 2 – Correlation for pseudocritical temperature



Figure 3 - Correlation for the Pitzer's acentricity factor

Correlation	Average	Minimum	Maximum	Standard	Residual	The standard
	_			deviation	variance of the	deviation of the
					regression	regression
					equation	equation
γ	0.732	0.561	1.026	0.142	—	—
$p_{pc}$ , MPa	0.4546	0.4406	0.4613	0.0059	0.0952	0.00212
$T_{pc}$ , K	216.281	192.119	253.074	17.346	2.0690	0.00665
ω	0.0305	0.0092	0.0628	0.0161	0.0000004	0.00062

Table 1 – Statistical estimates for regression equations (1) – (3)

$$p_{pc} = 4.8790^{\pm 0.0009} - 0.4877^{\pm 0.1068} \cdot \gamma -$$

$$-0.049739^{\pm 0.0685} \cdot \gamma^{2},$$

$$T_{pc} = 77.67^{\pm 0.15} + 254.42^{\pm 17.27} \cdot \gamma -$$
(2)

$$-85.62^{\pm 11.08}\cdot \gamma^2$$
 ,

$$\omega = -0.0811^{\pm 0.000} + 0.1898^{\pm 0.0075} \cdot \gamma - -0.0492^{\pm 0.0048} \cdot \gamma^2 .$$
(3)

Here and below, in the regression equations, the values of pseudocritical pressures and temperatures are presented in MPa and K.

The coefficient of determination for all regression equations exceeds the value of 0.99, which indicates the insignificance of the random component of the residual variance of the regression equation. Table 3 shows the statistical characteristics of the sample and estimates of the residual variance and the corresponding standard deviation of the regression equations (1)–(3). The width of the confidence interval for the quadratic term in the regression equation for pseudocritical pressure is larger than its value, so it is insignificant with the accepted 95 % confidence level. Linear dependences without power terms are much more resistant to argument errors, therefore, for pseudocritical pressure, it is reasonable and statistically justified to use linear regression of the form

$$p_{pc} = 4.8494^{\pm 0.0010} - 0.4141^{\pm 0.0342} \cdot \gamma .$$
 (4)

Comparison of the calculated and experimental data shows that the use of new correlations corrected for the content of nitrogen, carbon dioxide, and hydrogen sulfide in the cubic Soave–Redlich–Kwong equation provides an estimate of the supercompressibility factor with sufficient accuracy for practical purposes [14].

#### Calculation of bottomhole pressure in a well

To describe the distribution of gas pressure in the wellbore, for simplicity, a barometric formula is often used, which relates bottomhole pressure to wellhead pressure and has the form [7]:

$$p_{wb} = p_h \exp\left[\frac{0.03415\,\gamma L}{z}\right],\tag{5}$$

where  $p_{wb}$  is the bottomhole pressure;  $p_h$  is the working pressure at the wellhead; L is the depth of the well; z is the average value of the gas compressibility factor in the wellbore;  $\gamma$  is the relative density of the gas.

The so-called average supercompressibility factor is determined for the average values of pressure  $p_m$  and temperature  $T_m$ , calculated by the formulas:

$$p_{m} = \frac{2}{3} \left[ p_{wb} + \frac{p_{wb}^{2}}{p_{wb} + p_{h}} \right], \tag{6}$$

$$=\frac{I_{wb}-I_h}{\log\frac{T_{wb}}{T_h}},$$
(7)

where  $T_{wb}$ ,  $T_h$  are the temperatures at the bottomhole and wellhead, respectively.

 $T_m$ 

The system of equations (5)–(7) is supplemented by a procedure for calculating the gas supercompressibility factor and is solved relative to the bottomhole pressure by numerical methods.

In what follows, there are used the Soave– Redlich–Kwong equation of state and correlations (1)–(3) for pseudocritical pressure and temperature and the acentricity factor to calculate the supercompressibility factor. The accuracy of the bottomhole pressure calculation will depend on the accuracy of measuring pressure and temperature at the wellhead, the temperature at the bottom of the well, the accuracy of determining the relative density of the gas, and the error introduced by the regression equations.

The impact of input data errors on the bottomhole pressure calculation result using the barometric formula was assessed using the Monte Carlo method using the example of measuring the pressure distribution in two gas wells after they were stopped and the bottomhole pressure stabilized. Pressure and temperature measurements were carried out with high accuracy downhole instruments with an absolute error of pressure measurement of no more than 0.015 MPa and temperature of no more than 0.15 K. It was assumed that the standard deviation in determining the relative density of the gas was 0.005, in determining the nitrogen content -1.7 %, when determining the content of carbon dioxide - 0.27 %. The well gases did not contain hydrogen sulfide. Variations in the calculation of pseudocritical parameters and the acentricity factor of the gas corresponded to the confidence intervals of the coefficients of the regression equations (1)–(3).

Figure 4 illustrates a comparison of the pressure data actually measured in the wells with those calculated by the barometric formula with the corresponding confidence intervals, estimated after 50,000 Monte Carlo attempts. The relative width of the reliability interval at the last measurement point for Well 17 was 1.3 %, and for Well 32 - 2.8 %.



Figure 4 – Bottomhole pressure calculation results by barometric formula using new regression dependencies for pseudo-critical gas properties

The sensitivity analysis of variance (Table 2) of the simulation results showed that in both examples, about 70 % of the errors was due to the variation in determining the pseudocritical temperature. The density of the gas also made a significant contribution to the total variation. Although the accuracy of its determination in laboratory conditions was high, the frequency of its determination in the well could cause already noticeable system errors.

Origin of ormon	Contribution to variance		
Origin of error	Well 17	Well 22	
Relative gas density	0.27406	0.27697	
Critical pressure	0.00063	0.00020	
Critical temperature	0.71677	0.71389	
Acentricity factor	0.00044	0.00422	
Wellhead pressure	0.00106	0.00134	
Wellhead temperature	0.00006	0.00001	
CO <sub>2</sub> content	0.00110	0.00181	
N <sub>2</sub> content	0.00175	0.00133	
Other	0.00412	0.00024	

 Table 2 – Contribution of input parameters errors

 to the variation of bottomhole pressure calculation

# Estimation of gas reserves using the material balance method

To assess the impact on the accuracy of determining the final producing gas reserves by the dependence of the reduced reservoir pressure p/z on the cumulative production  $V_{prod}$ , a real example of a gas

facility with a pronounced gas development mode was selected (Figure 5). Reservoir pressures in the wells operating the facility were measured by downhole instruments with an error not exceeding 0.015 MPa.

For the first example, the approximation of the dynamics of the measured reservoir pressure with a complete system of material balance equations using the MBE (Gas field material balance) program [1] with minimization of the residual error by the dichotomy method made it possible to estimate the initial gas reserves for the object at 743.43 million m<sup>3</sup>. The residual root-mean-square error of the material balance model was 0.0815 MPa, and the coefficient of determination of the model was 0.9993, which clearly indicates the pure gas mode of deposit development and the reliability of gas reserves estimates.

In practice, a simplified material balance model is often used to determine gas reserves in a deposit. So, for a closed gas reservoir, when there is no external water inflow, the pore gas-saturated volume does not change, the formation temperature is constant, the material balance is written using the generalized Clapeyron– Mendeleev law in the form:

$$\frac{p_t}{z(p_t,T)} = \frac{p_{in}}{z(p_{in},T)} - \frac{p_{st}}{z(p_{st},T_{st})} \frac{V_{prod.t}}{V_{por.ini}}, \quad (8)$$

**T** 7

where  $p_{sb}$ ,  $T_{st}$  are pressure and temperature for standard conditions for accounting of produced gas;  $V_{prod,t}$  is the current accumulated volume of produced gas at time *t*;  $p_{in}$  is the initial reservoir pressure;  $z_{in}$ ,  $z_b$ ,  $z_{st}$  are gas supercompressibility factor at initial and current



Figure 5 – The results of approximation of reservoir pressure dynamics by the material balance model in the gas operation mode of the deposit (1<sup>st</sup> reservoir)



Figure 6 – Approximations of the dynamics of reduced reservoir pressure by a linear regression equation (1<sup>st</sup> reservoir)

reservoir conditions and at standard conditions, respectively;  $p_{in}$ ,  $p_t$  are initial and current reservoir pressure, respectively; *T* is reservoir temperature;  $V_{por.ini}$  is the initial pore volume occupied by gas.

From equation (8) it follows that the initial reserves in the reservoir can be determined by the formula:

$$Reserves = -\frac{a}{b} , \qquad (9)$$

where a, b are the parameters of the linear regression dependence

$$\frac{p_t}{z(p_t,T)} = a + b V_{prod.t} \quad . \tag{10}$$

Formula (9) is the basis for determining the producing gas reserves in the gas mode of development by the dependence of the reduced reservoir pressure p/z on the volume of gas produced (Figure 6).



Figure 7 – Results of approximation of the reservoir pressure dynamics by the material balance model in a mixed reservoir operation mode (2nd reservoir)

The coefficients of the linear regression equation for the dynamics of the reduced reservoir pressure (Figure 6), estimated by the least squares method with a probability of 95 %, have the value

$$a = 15.548 \pm 0.225,$$
  

$$b = -0.02083 \pm 0.00001,$$
(11)

and the initial gas reserves in the reservoir were  $Reserves=746.15\pm10.85$  million m<sup>3</sup>.

The residual root mean square error for reservoir pressure is 0.0890 MPa, and the coefficient of determination of the model is 0.9992, which confidently indicates the pure gas mode of deposit development. The statistical characteristics of the quality of the linear regression equation are slightly inferior to the characteristics of the material balance model, which additionally takes into account the compression of the pore space and bound water in the system of equations in the gas regime. And to a large extent, this is also due to the good quality of reservoir pressure measurements and the almost complete absence of other energy sources of gas movement in the reservoir, except for its elastic energy reserve.

The dispersion sensitivity analysis (Table 3) of the results of calculating the initial gas reserves by the dependence of the reduced reservoir pressure on the cumulative gas production showed that for this example, more than half of the possible error in determining the gas reserves was associated with the accuracy of measuring the value of the cumulative gas production. Note that the contribution from the uncertainty of the critical temperature is noticeably higher than the contribution from the uncertainty of the critical pressure. This is explained by the fact that in one of the coefficients of the Redlich–Kwong equation of state, the critical pressure – only the first power.

	Table 3 – Contribution of input data errors
to	the variation in determining the initial reserves
	of the gas deposit (1st reservoir)

Origin of error	Contribution to variance	
Accumulated production	0.5914	
Critical temperature	0.3587	
Acentricity factor	0.0014	
Critical pressure	0.0013	
Other	0.0472	

The second example of reservoir pressure dynamics (Figure 7) illustrates the influence of an active aquifer on the reliability of reserves determination based on the dependence of reduced reservoir pressure on cumulative production. Reservoir pressures in the wells operating the facility were calculated using the barometric formula, based on the pressure at the shut-in wellhead. The pressure was measured by manometers, accuracy class 0.4.

For the second example, the approximation of the dynamics of the measured reservoir pressure by a system of material balance equations with minimization of the residual error by the MBE (Gas field material balance) program [1] gave an estimate of the initial gas reserves for the object at 391.51 million m<sup>3</sup>. The potential of the aquifer estimated is at 8.366 million m<sup>3</sup> and its productivity index at  $5.176 \cdot 10^{-5}$  million m<sup>3</sup>/(MPa · day). The residual rootmean-square error of the material balance model was 0.589 MPa, and the coefficient of determination of the model was 0.941.

If the assessment of gas reserves in this deposit is carried out based on the approximation of the dynamics of the reduced reservoir pressure by a linear regression equation (Figure 8), a high coefficient of determination of 0.9379 attracts attention. Formally, this gives reason



Figure 8 – Approximation of reduced reservoir pressure dynamics by linear regression equation (2nd reservoir)

to consider the use of a linear approximation statistically justified – the random share in the variation is insignificant. High, and statistically significant, values of the coefficient of determination will be typical for any deposit. Gas production, even with a highly active aquifer, objectively leads to a decrease in reservoir pressure in the deposit, which later manifests itself in the form of a correlation between reservoir pressure and production, which suppresses the random component of this dependence. Therefore, a high coefficient of determination for the relationship between reduced reservoir pressure and cumulative gas production is a weak criterion for concluding that it is possible to estimate gas reserves using a linear model.

The residual root mean square error of the linear model for reservoir pressure was 0.820 MPa. When comparing with the results of approximation by the material balance equations, taking into account the formation water activity, we pay attention to the difference between the residual errors of 0.820 and 0.589. According to Fisher's test, this difference is statistically significant. While the coefficients of determination of both models are little different and statistically significant and do not give the advantage of one model.

The coefficients of the linear regression equation for the dynamics of the reduced reservoir pressure in the second example, estimated by the least squares method, with a probability of 95 % have the value as follows

$$a = 13.680 \pm 1.103,$$
  

$$b = -0.02677 \pm 0.00007,$$
(12)

and the initial gas reserves in the reservoir are estimated as Reserves =  $510.99 \pm 42.64$  million m<sup>3</sup>.

The wide confidence interval for the linear model is mainly due to the high variance of reservoir pressure measurements relative to the average trend. The reason for this is the system errors in the technology for determining reservoir pressure in the conditions of an active aquifer, which is much smaller for this device, the contribution to the overall variance of the accuracy of measuring wellhead pressure and volumes of produced gas, and the participation of uncertainties in correlations for pseudocritical parameters and the gas acentric factor is completely negligible.

#### Conclusion

An analysis of the influence of uncertainties in the empirical correlations of pseudocritical characteristics and the acentricity factor of natural gas with its density on real examples has shown that only when calculating reservoir pressure using the barometric formula, their influence is comparable to the contribution of instrumental errors in pressure and temperature measurements. Uncertainties in the use of correlations in estimating gas reserves based on the dependence of the reduced reservoir pressure p/z on the volume of gas produced are absorbed by instrumental and system errors in measuring reservoir pressure and gas production.

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# Ризики емпіричних кореляцій для псевдокритичних властивостей природного газу

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Оцінено вплив невизначеностей при використанні емпіричних кореляцій псевдокритичних властивостей природного газу з його густиною на результати визначення запасів газу та вибійних тисків.

Моделювання на прикладах розрахунку вибійного тиску в газовій свердловині та створення матеріального балансу газового покладу показали, що їх вплив у загальну похибку може бути зіставним із внеском інструментальних похибок лише при високоточних вимірюваннях тисків і температур. При визначенні коефіцієнта надстисловості газу за його псевдокритичними властивостями близько 70 % похибок зумовлено варіацією псевдокритичної температури.

**Ключові слова:** коефіцієнт стисливості, матеріальний баланс, метод Монте-Карло, фактор ацентричності.