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A SUMMARY OF METHODS ON CALCULATIONS OF GAS  
DENSITY

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Lecturer: Mr. M. R. Pritchard,  
Sarasota Automation Ltd.

Authors: T. Cousins and P. Mason

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A SUMMARY OF METHODS ON CALCULATIONS OF  
GAS DENSITY

BY

T.COUSINS and P. MASON.

(1.0) INTRODUCTION

The objective of this paper is to review some of the current methods of calculating density to achieve mass flow measurement. Most flow-meters used for gas measurement, orifice plates, turbine meters, vortex meters etc., measure ACTUAL VOLUMETRIC FLOW, or more specifically ACTUAL FLOW VELOCITY. The value of product is in its Mass as this is an 'inviolable' quantity whereas actual volume flow is different for different conditions such as pressure and temperature. Density must therefore be measured to be combined with the actual volume flow to give mass flow.

There are four methods of obtaining density for gas :-

- a) A fixed estimated value (commonly used in compressed air, steam systems and gas supply to consumers)
- b) Simple checking, by taking a sample of the process fluid and measuring its properties in the laboratory.
- c) On line densitometry, mainly vibrating spool densimeters or gas chromatography.
- d) Calculation of density by pressure and temperature inputs.

The purpose of this paper is to concentrate on the pressure and temperature method of density measurement with emphasis on summarising the methods of correcting for compressibility.

(2.0) REVIEW OF OTHER METHODS

Before discussing the p-T method it is worth reviewing the other methods as it is sensible practice to use two (or more) methods of density determination as a check. Particularly as polling 2 from 3 in fiscal measurement will add greatly to the confidence of the density measured.

(2.1) FIXED ESTIMATED VALUE

Obviously with varying pressures and temperatures such a method will be inaccurate, although it is useful for 'fallback values' and alarm limits. Further if temperature and pressure are reasonably constant it is a useful check for other methods. It is interesting to note that gas is metered uncorrected to households, taking an average annual temperature and an assumed regulated pressure for density calculation. While individually the financial value is small, the percentage loss to the consumer is the same as the gas producers if they used the same method (in the U.K., in an average year British Gas are between 3 and 5% safe in their predictions)

(2.2) SAMPLE CHECKING

For this method samples of the gas have to be removed from the pipeline and taken to the laboratory for analysis. This can be done in a variety of ways, such as the buoyancy gas balance, recording gravitometer, momentum gravitometer etc. The problems with this method are ensuring the test conditions are the same as the flowing conditions (if not they will have to be related back by calculation with consequent errors), how representative is the sample and finally it does not represent a continuous measurement. It is however a very useful comparison for the on-line density and p-T method.

(2.2) ON LINE DENSITOMETRY

There are several methods for on line densitometry, the vibrating spool/plates method and gas chromatography being the most common. A typical vibrating spool densitometer is shown in FIG 1. The spool is set in vibration at resonance in a circumferential mode. Gas passes around the spool changing the mass at the surface, which in turn effects the resonant frequency (f) in the form:-

$$f = \sqrt{K / (M_s + M_g)}$$

Where K is the spring rate,  $M_s$  is the spool mass and  $M_g$  the local mass of gas. Obviously for maximum sensitivity the mass of the spool must be as low as possible compared to the gas mass. The obvious advantages of the system are direct measurement of density, to in many cases a very high order of uncertainty (better than 0.3%)

There are a number of disadvantages to densitometers:-

1) It is difficult to ensure that the sample passing through the densitometer is representative of the fluid passing through the meter. This is alleviated somewhat by different methods of positioning the densitometer.

2) Reliability of the densitometer due to fouling (with the problem of being unable to tell when errors occur)

3) Uncertainty of Velocity of sound correction of certain gases.

On line Gas chromatography also can be used to give good answers of density however it suffers the problems of:-

a) Varying density product will give errors (if faster than sample time)

b) Cost of the instrument.

c) Lack of ruggedness.

Both methods can give answers better than p-T methods but because of the problems can be considered suspect on their own. A sensible approach would seem to use either or both in conjunction with the p-T methods to be described in Section 5. -

### (3.0) DENSITY REQUIREMENTS

As previously stated density is required to obtain mass flow as most flowmeters are volumetric.

The basic flow equations to be satisfied are:

$$\text{ORIFICE PLATE: } \dot{m} = K\sqrt{\Delta P \times e}$$

$$\text{TURBINE/VORTEX: } \dot{m} = KFe$$

A point worth noting is that errors in density measurement for an orifice plate are halved when flow is measured. The positions of measurement of pressure and temperature are usually downstream of the orifice and then corrected back to the orifice conditions. Fig 2. Measuring pressure at the downstream is useful as the jet mixes together any stratified gas, to give a better density distribution. It is also important obviously that the temperature is related to that at the orifice. Recent work seems to show that significant temperature differences are seen at the orifice due to the fluid mechanism not being isothermal or isentropic. This will impact the density and compressibility calculations.

(4.0) ACCURACY REQUIREMENTS

Measurement of gas is following the trend of all flow measurement in that there is a continual push for greater perceived accuracy. However many of the gas installations are still orifice plates for which there is very little opportunity to improve on the basic orifice plate uncertainty, other than by calibration of each orifice individually. The drive has therefore concentrated on peripheral measurements such as temperature, pressure and density. The problem here is that these errors are now considerably smaller than the uncertainty of orifice plate measurement and so the improvements in uncertainty are becoming less realistic. On line densitometers can meter within  $\pm 0.2$  to  $\pm 0.3\%$  subject to installation conditions, giving an orifice plate a  $\pm 0.15\%$  mass flow error due to density. Thus for calculation of density in general it is required that this be better than  $0.3\%$ . Now pressure measurement error is  $\pm 0.1\%$  FSD and assuming temperature errors to be  $\pm 0.05\%$  FSD then using RMS errors the uncertainty of measurement of all other errors for p-T calculation must be better than  $\pm 0.26\%$  to be better than densitometry. The largest error will come from the calculation of compressibility.

(5.0) DENSITY CALCULATION

The density for a real gas is given by:-

$$\rho = P \times M_w / ZRT$$

The compressibility factor is used to convert the equation from an ideal gas equation to a real gas. For an ideal gas  $Z = 1$  and for a real gas it varies dependant upon temperature, pressure, gas and mixture. There are a number of methods of calculating the compressibility either using equations of state (Redlich - Kwong) or interpolations of data (NX19). Each has a specific application and an area over which it is effective. Obviously there is a large amount of research currently going forward with the objective of achieving a universal law.

(6.0) COMPRESSIBILITY CORRECTIONS

(6.1) COMPRESSIBILITY - FACTOR DIAGRAMS

One of the earliest methods for compressibility was to use equations of state determined from generalised compressibility diagrams. The two main methods are the Nelson-Obert diagram and the Edmister-Pitzer diagram. Nelson-Obert diagrams are based on two parameter reduced temperature and pressure diagrams FIG 3, based on 26 single component gases. Reduced pressure  $P_r = P/P_c$  and reduced temperature  $T_r$  is defined as  $T/T_c$ , suffix: C being at the critical conditions e.i. the point of equal specific volume. For these gases the smoothed curves fit to within 1%. Once other gases are used the error increase to 2% for compressibility factors of 0.6 and above and up to 6% for factors between 0.3 and 0.6. Edmister-pitzer diagrams improve the prediction by introducing a third parameter factor ( $\omega$ ) called the acentric factor, based on how spherical the nature of the molecular force field of the gas. For simple fluids such as argon  $\omega = 0$ . They assumed that fluids with the same pVT relationship have the same ( $\omega$ ), and the deviation is linear to adjust ( $\omega$ ) for the nature of the fluid then  $Z = Z_0 + \omega Z_1$ , where  $Z_0$  is the simple compressibility and  $Z_1$ , the deviation. The data can be derived from two diagrams FIG 4 and from the equation

$$\omega = (3 \log(P_c/14.7) / 7 (T_c/T_b - 1)) - 1$$

It is possible to obtain accuracies of better than  $\pm 1\%$  over  $Z$  ranges of 0.6 - 1.0 for non-polar gases. A version of this method called the corresponding states equations is used by British gas. Combined with accurate data this method gives a low uncertainty for natural gas.

(6.2) CALCULATION METHODS

(6.21) REDLICH-KWONG EQUATIONS

The Redlich-Kwong equation is a two constant equation of state that may be adapted to calculate compressibility from  $T_r$  and  $P_r$ . Compressibility is given by

$$Z = 1 + A \frac{-AB}{A+Z} + \frac{A^2 B}{A^2 + Z^2}$$

where

$$A = \frac{0.0867 P_r}{T_r} \quad B = \frac{4.934}{T_r^{1.5}}$$

As the equation is non-linear it has to be solved iteratively, Newtons method being the simplest. FIG4 shows the deviation of  $Z$  with varying  $T_r$  and  $P_r$  for methane. At low pressures agreement with actual is good, better than 0.5%, but with increasing pressure and temperature the error increases significantly. Substantial modifications have been made to the basic theory by both Gaz de France and Ruhr gas but in general the equations are still not good at predictions at pressures above 60 bar absolute.

(6.22) BENEDICT-WEBB-RUBIN

The BWR equation is an 8 parameter equation of state. Compressibility can be derived from the two equations:

$$P = RTe + (B_0 RT - A_0 - C_0/T^2)e^2 + (bRT - a)e^3 \dots$$

$$+ Ce^3(1 + \gamma e^2) \sqrt{T^2} - \delta e$$

$$e = \frac{PM_w}{ZRT}$$

$A_0, B_0, C_0, a, b, C, \gamma, \alpha$  are empirical constants specific to the fluid concerned. This equation appears to have a good range of application although above 62 bar the deviation again appears to increase, errors of over 0.5% being likely.

(6.23) OTHER EQUATIONS OF STATE

There are a number of less commonly used equations of state such as the Peng-Robinson equation which is similar to the R-K equations. Emphasis seems to be on improving and 'honing' down the already proved equations to obtain improved uncertainty, by adding empirical corrections.

(6.3) INTERPOLATION METHODS (EMPIRICAL)

There are a number of empirical methods for determination of gas compressibility. They are based on the collection of experimental data, and then the production of curve fits to meet the data.

(6.31) AGA3 NX19

The American gas association, rather than use equations of state undertook an extensive program of experiments to produce universal data. Several hundred experimental points were taken and a curve fit derived to give super-compressibility  $F_{PV} = \sqrt{1/Z}$  where  $Z$  is compressibility. The square root function comes from the initial requirement being for orifice plates. The immediate problem with the equations is that for all values of temperature a pressure of 1.01325 bar a. leads to unity, i.e.  $Z = 1$ . This is not acceptable as it should only lead to 1 for an ideal gas. The basic curve fit for the equations are:-

$$F_{PV} = \frac{\sqrt{B/D - D + n/3\pi}}{1 + (0.00132/\tau^{3.25})}$$

Where

$$B = \frac{3 - mn^2}{9m\pi^2} \quad m = f(\tau)$$
$$D = (b + (b^2 + B^3)^{\frac{1}{2}})^{\frac{1}{3}} \quad n = f(\tau/m)$$
$$b = \frac{9n - 2mn^3}{54m\pi^3} - \frac{E}{2m\pi^2} \quad \pi = f(P)$$
$$\tau = f(T)$$

E = NX19 Table Extrapolation.

The tables were derived for a lean natural gas of specific gravity 0.6 containing no dilutants. T and P corrections were applied for gases with other gravities, and for gases with nitrogen and carbon dioxide additives. The following conditions over which NX19 is recommended are temperatures 230 to 390°K, pressure 340 bar and up to 15% nitrogen and carbon dioxide. This allows for compressibility determination for SG in the range 0.554 to 1.000.

To correct for the basic deficiencies of the concept, there are at least 6 different proposed corrections.

- 1) Texas Eastern Transmission Corp/British Gas proposed a modification given by  $Z_{PT} = Z_{AGA} \times Z_T$  where PT represents corrected value, AGA is NX19 value and T is temperature correction at P= 1.01325bar a.
- 2) C.E.R.G. proposed a version:-  $Z_{PT} = Z_{AGA} \times Z_S^2 / Z_\eta$  where S refers to P=1.01325bar a. and 15.55°C and  $\eta$  refers to P=1.01325 bar a. and 0°C.
- 3) Herning and Wolowski (Ruhr Gas) proposed two versions, one based on translocation of the scale, implying that  $Z_{AGA}$  is unity for P=0 rather than 1.01325bar a.
- 4) They also proposed that  $Z_{PT} = Z_{AGA} \times Z_\eta$
- 5) Gaz de France proposed that  $Z_{PT} = Z_{AGA} \times Z_S$
- 6) A further concept idea by Gas de France the change would be

$$Z_{PT} = Z_{AGA} - (1 - Z_T)$$

This is not based on scientific evidence but seems to give reasonable correction up to 80bar a.

Corrections 2, 3 and 4 give answers at P=1.01325bar a. which is not correct.

These corrections all show a reduction in error but they do not correct the inherent defects in the basic empirical relation determined from experimental error.

The NX19 equation is very specific to natural gas and cannot be used for other gases. In general the NX19 equations do not seem to perform as well as some other methods except at very high pressure, above 82bar and high SG, although within specific ranges of pressure, temperature methane content the performance can be very impressive, RMS errors of the order of 0.1%

#### (6.32) AGA 8 GRI

The latest method of compressibility calculation is the GRI equations now incorporated in AGA 8. It is a semi-empirical method based initially on an equation of state, with fine tuning from empirical data.

The basic equation is given by  $Z = Z_0(T_r, \rho_r) + \delta Z_\gamma(T_r, \delta_r)$

where  $\delta$  is a parameter similar to the acentric factor.

$\rho$  = molar density,  $\epsilon$  = energy parameter and  $\sigma$  separation, parameter obtained from :-

$$T_r = KT/\epsilon \quad , \quad \epsilon_r = \epsilon \sigma^3$$

$$\sigma^3 = 0.3189/\rho_c \quad , \quad \epsilon/K = T_c/1.2593, \quad t = (T_r)^{-0.5}$$

$Z_0$  was determined from selected experimental data, second virial coefficient, enthalpy departure and vapour pressure data for methane, giving

$$Z_0 = 1 + (a_1 + a_2 t + a_3 t^2 + a_4 t^3 + a_5 t^4 + a_{27} t^5 + a_{17} t^7 + a_{16} t^8) \epsilon_r \\ + (a_6 t + a_7 t^4 + a_8 t^5 + a_{18} t^{10}) \epsilon_r^2 + (a_9 t + a_{10} t^2 + a_{11} t^3) \epsilon_r^3 \\ + (a_{12} t^2 + a_{13} t^6) \epsilon_r^5 + a_{14} t^6 \epsilon_r^2 + (1 + a_{15} \epsilon_r^2) \exp(-a_{15} \epsilon_r^2)$$

$Z_8$  is found similarly with data from ethane, propane, nitrogen, carbon dioxide etc. up to 11 constituents and is given by:-

$$Z_8 = (a_{19} t + a_{20} t^4) \epsilon_r + (a_{23} + a_{24} t^4) \epsilon_r^2 + (a_{25} t^4 + a_{26} t^5) \epsilon_r^3 \\ + a_{21} t^2 \epsilon_r^5 + a_{22} t^6 \epsilon_r^2 (1 + a_{15} \epsilon_r^2) \exp(-a_{15} \epsilon_r^2)$$

$a_i$  in the equation are equation of state constants.

While this equation set is still relatively new it does appear to be giving high quality answers. For general natural gas the compressibility may be calculable to within a 0.3% absolute deviation up to 150bar a. Perhaps however its greatest feature is that it does have more general application than the other methods, from pure gases through to complex mixtures.

### (6.33) IUPAC TABLES

The international union for Pure and Applied Chemistry (IUPAC)

have produced tables for a variety of gases. In particular they

have produced useful extrapolation of tables for Ethylene and high

and low pressures. For low pressure this takes the form  $Z = \sum_{i=0}^2 \sum_{j=0}^{\infty} B_{ij} T^{-j} \epsilon^i$

Where the coefficients are obtained from IUPAC tables.

### (7.0) SUMMARY

The paper is a very loose summary of the methods for calculating density,

on line. It misses out several methods of compressibility calculation

such as Standing-Katz and Vennix-Kobayashi. Overall the picture that

emerges is that all of the methods have use in different applications,

and maybe a manufacturer of flow computers has to include them all in

software with a preference selection based on pressure, temperature content, density range combined with mind reading software for personal preference. Perhaps the latest method the GRI will allow a rationalisation if in the end it is shown to have the range it appears to have.

From a practical stand point it would seem more suitable to combine two or preferably three methods, calculation, direct density by densitometer and density by gas chromatography to obtain a reliable answer for density. A summary of the limitations of the different methods are below based on the references given.

METHOD OF COMPRESSIBILITY DETERMINATION	SENSIBLE PRESSURE RANGE BAR	PROCESS FLUID	MINIMUM ERROR	OVERALL ERROR *
NELSON - OBERT		Polar Gases	+ - 1%	+ - .4 - 6%
EDMISTER - PITZER		Polar & Non-Polar Gases	+ - 1%	+ - 3%
REDLICH-KWONG **	50 bar A.	Various	+ -0.5%	+ - 2% 50-100bar A
BENEDICT-WEBB-RUBIN	80 bar A	Various	+ -0.4%	+ - 1% *** with offset
AGA3 NX19	100bar A	Natural Gas & Dilutents	+ -0.5%	+ - 1% 100-150Bar A
AGA 8 GRI	150bar	All Gases	+ -0.15% for natural Gas	
IUPAC - low pressure		Ethylene	+ -0.2%	
STANDING-KATZ	150bar	Natural Gases	+ -0.6%	

\* A combination of offset and linearity errors have been combined

\*\* Depends on modifications

\*\*\* Reference 8 gives much better results <sup>+</sup>-0.2 up to 150 Bar A for Natural gas.

The results from all the references are subject to wide interpretation and so the table is necessarily broad in its error band. Also these errors are purely those obtained under 'ideal' experimental conditions and are likely to be larger under process conditions

(8.0) REFERENCES

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LIST OF SYMBOLS

$\dot{M}$	=	Mass Flow
$K$	=	Flow Constant
$\Delta P$	=	Orifice Differential
$\rho$	=	Density
$f$	=	Turbine/Vortex Frequency
$P$	=	Pressure of Fluid
$P_c$	=	Critical Pressure
$M_w$	=	Mole Weight
$R$	=	Universal Gas Constant
$Z$	=	Compressibility factor
$T$	=	Absolute Temperature
$T_c$	=	Critical Temperature
$T_B$	=	Boiling Temperature
$\omega$	=	Accentric Factor

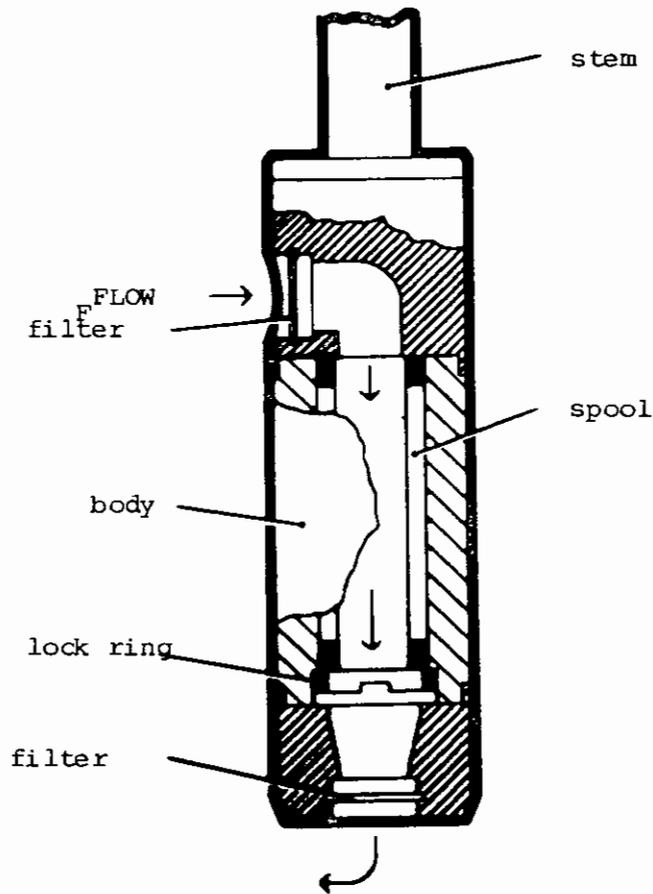


FIG. DENSITOMETER

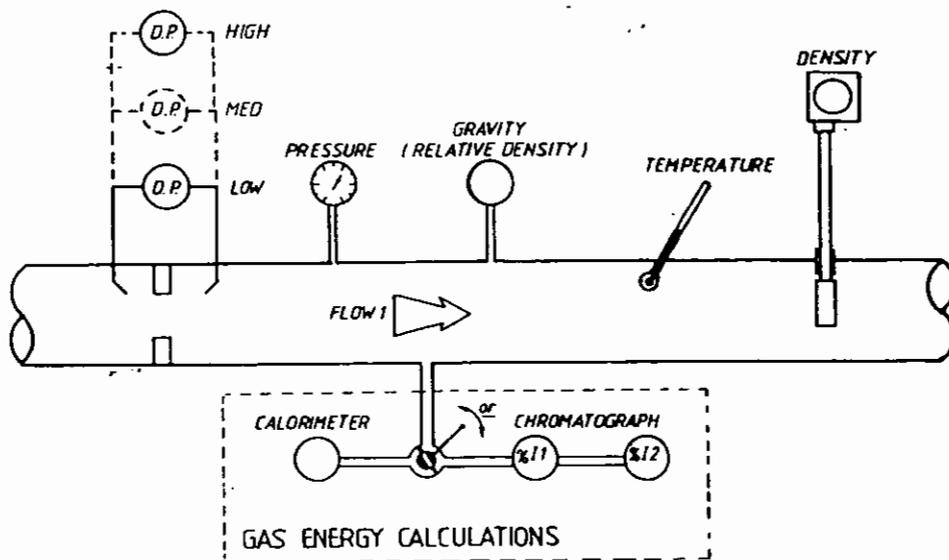


FIG.2 GAS ORIFICE INSTALLATION

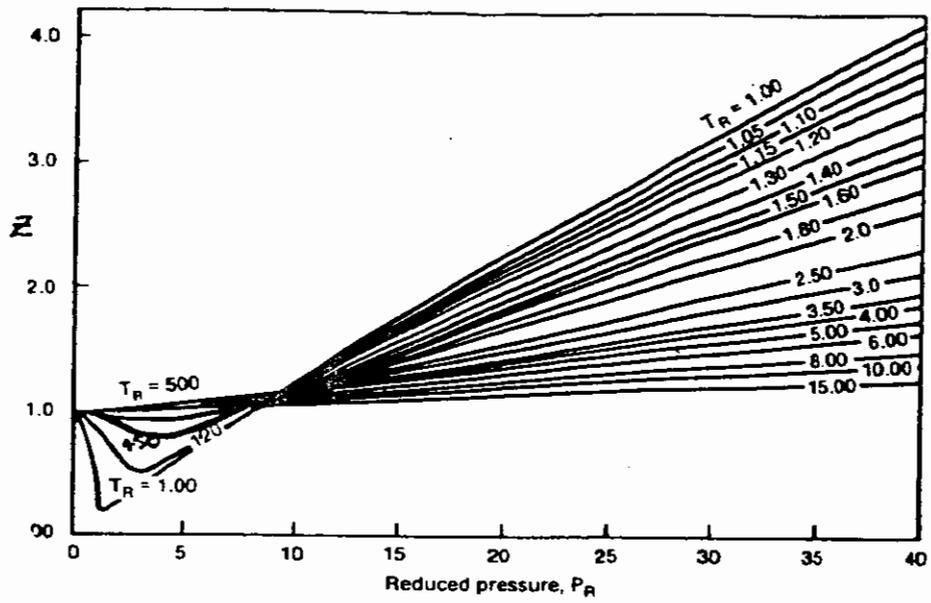


FIG. 3 NELSON-OBERT COMPRESSIBILITY DIAGRAM

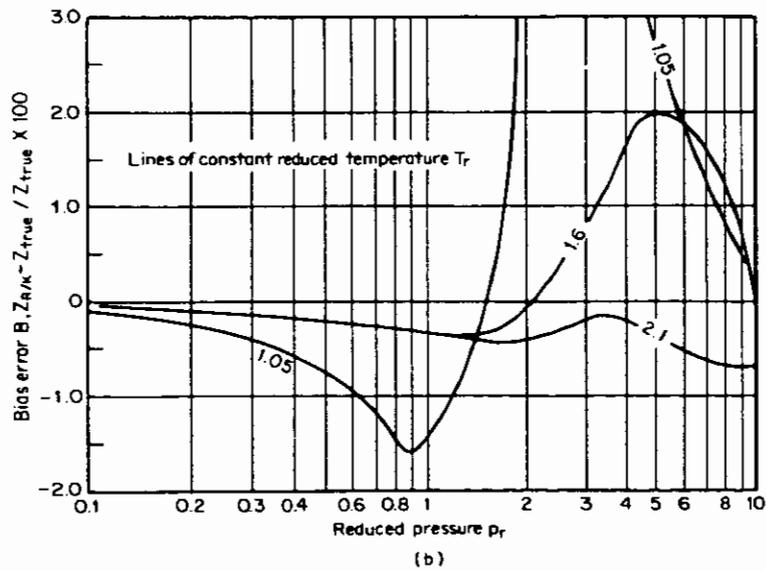


FIG. 4 ERROR CURVES FOR METHANE FOR THE BASIC REDLICH-KWONG EQUATION