Compressibility Factors for the Hydrogen-Methane System

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TABLE 1. *B* COEFFICIENTS FOR METHANE-HYDROGEN MIXTURES

		10.0°C (50°F)	−17.8°C (0°F)	−45.6°C (−50°F)	−73.3°C (−100°F)	−101.1°C (−150°F)
Methane	B_1	−0.46042 E 02	−0.60029 E 02	−0.80560 E 02	−0.10126 E 03	−0.14232 E 03
	B_2	0.11411 E 04	0.14997 E 04	0.31511 E 04	0.16389 E 04	0.51228 E 04
	B_3	0.25794 E 06	0.24030 E 06	0.10098 E 06	0.53139 E 06	
	B_4	−0.19851 E 08	−0.18702 E 08	−0.13530 E 08	−0.45054 E 08	
	B_5	0.66544 E 09	0.62153 E 09	0.54037 E 09	0.12552 E 10	
	P max	48.26	38.29	39.60	34.93	2.32
	ρ max	0.0176	0.0179	0.0201	0.0214	0.0023
Gas A	B_1	−0.30204 E 02	−0.39655 E 02	−0.52436 E 02	−0.68930 E 02	−0.89321 E 02
	B_2	0.22134 E 04	0.24769 E 04	0.27602 E 04	0.31593 E 04	0.14805 E 04
	B_3	−0.50718 E 05	−0.62322 E 05	−0.63220 E 05	−0.19978 E 05	
	B_4	0.35533 E 07	0.37561 E 07	0.34716 E 07	−0.24465 E 07	
	B_5				0.19077 E 09	
	P max	48.81	35.47	31.05	39.53	3.28
	ρ max	0.0173	0.0164	0.0177	0.0214	0.0031
Gas B	B_1	−0.14159 E 02	−0.24747 E 02	−0.32643 E 02	−0.43427 E 02	−0.61605 E 02
	B_2	0.12499 E 04	0.19556 E 04	0.17801 E 04	0.13473 E 04	0.19799 E 04
	B_3	0.40574 E 04	−0.44425 E 05	−0.12379 E 05	0.10069 E 06	
	B_4	0.13232 E 07	0.25316 E 07	0.14654 E 07	−0.65044 E 07	
	B_5				0.19016 E 09	
	P max	47.89	41.07	31.54	41.39	4.61
	ρ max	0.0166	0.0170	0.0166	0.0214	0.0041
Gas C	B_1	−0.42822 E 01	−0.55844 E 01	−0.12148 E 02	−0.19991 E 02	−0.26329 E 02
	B_2	0.23452 E 04	0.10421 E 04	0.11955 E 04	0.12901 E 04	0.19173 E 04
	B_3	−0.17009 E 06	−0.83688 E 04	−0.10447 E 05	−0.45867 E 04	−0.48160 E 05
	B_4	0.66718 E 07	0.11152 E 07	0.10484 E 07	0.78601 E 06	0.17722 E 07
	P max	43.95	47.55	38.29	36.38	20.28
	ρ max	0.0151	0.0175	0.0171	0.0190	0.0148
Gas D	B_1	0.75910 E 01	0.52600 E 01	−0.34743 E 01	−0.78581 E 01	−0.28193 E 01
	B_2	0.96876 E 03	0.10633 E 04	0.62719 E 03	0.62057 E 03	0.67368 E 03
	B_3	−0.47928 E 05	−0.56241 E 05	0.42492 E 04	0.10649 E 05	0.25567 E 04
	B_4		0.25056 E 07	0.35310 E 06	0.13448 E 06	0.55003 E 06
	P max	49.10	42.82	37.85	37.37	34.27
	ρ max	0.0158	0.0157	0.0159	0.0178	0.0188

E—XX indicates power of 10.
P max is maximum pressure MPa.
ρ max is maximum density g mole/cm^3

Results of an investigation (Mueller, 1959) on the volumetric behavior of methane and four mixtures of methane and hydrogen were reported in this *Journal* by Mueller et al. (1961). The Burnett (1936) method was applied from +10° to −129°C at 28 deg. intervals to pressures as high as 48 MPa (7000 lb/sq. in. abs.). In the classical Burnett procedure, an isothermal series of pressure measurements is made as the gas is expanded from one cell into a second evacuated cell. A simple graphical limiting procedure developed by Burnett (1936) yields compressibility data. This procedure was used to obtain a table of smoothed compressibility factors for the studies of Mueller.

Significant improvements in the methods of analysis of Burnett data have since occurred: the direct method of Hoover et al. (1964) and the application of least-squares adjustable parameters calculations by Hall (1967) and Hall and Canfield (1970). The experimental procedure for the Burnett experiment has also been improved by the development of the isochorically coupled method by Pope et al. (1972). Experimental equipment has undergone major modifications (Ruska et al., 1973). All of these improvements were utilized by Pope (1971) in his study of the virial coefficients of argon, methane, and ethane (Pope et al., 1973).

The multidimensional, nonlinear least-squares regression analysis has been applied here to the data of Mueller et al. (1961). Detailed tables of these results are in the thesis of Pope (1971), available from University Microfilms.

The parameters obtained may be used to interpolate with respect to density along the isotherms. The compressibility factor is defined by

$$Z = 1 + \sum_{k=1}^{n} B_k \rho^k$$

where the *B*'s are in units of cubic centimeters per gram

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TABLE 2. EXPERIMENTAL GAS COMPOSITIONS

Mole %	CH_4	A	B	C	D
CH_4	99.7	79.4	64.5	43.1	21.7
H_2	0.0	20.2	35.1	56.5	78.0
N_2	0.2	0.3	0.3	0.2	0.2
Others	0.1	0.1	0.1	0.2	0.1

mole, and the density ρ is gram mole per cubic centimeters. When all possible errors are considered, the Z values are probably accurate to $\pm 0.10\%$.

The parameters B are given in Table 1. Note that the values of B coefficients are given for numerical precision, and the calculated Z should be rounded. The experimental gas compositions are given in Table 2. The maximum experimental pressure is also listed in Table 1; extrapolation to higher pressures is questionable. The $-129°C$ isotherms were not reanalyzed because there were too few points along these isotherms to justify the analytical method being used.

The values for methane are included in Table 1; however, the authors recommend that the equation of state by Vennix and Kobayashi (1969) be used for more precise computations on methane.

These data should be useful for present day coal gasification studies.

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A Simple Method of Calculating Effectiveness Factors for Heterogeneous Catalytic Gas-Solid Reactions

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For many practical purposes the design of a catalytic reactor may have to be made with a lack of precise information on the physical and chemical properties of reactants and products. Under such circumstances use of an elaborate model to predict the catalyst effectiveness may not be warranted and a simpler approach should suffice. This note presents a simple method of general utility for calculating effectiveness factors. The method which gives very good agreement with more exact solutions is similar to that recently noted by Aris (Aris, 1975, Georgakis and Aris, 1975). That method, however, involves a graphical solution whereas the method proposed in this note, being confined to isothermal or near isothermal conditions, requires (in combination with the asymptotic approximation) only the solution of a simple algebraic equation to determine particle effectiveness for any particular value of the Thiele modulus.

Many catalytic chemical reactions can be represented by the Langmuir-Hinshelwood model which is described by the general expressions

$$r = \frac{(kC_s^n)\, C^n}{[1 + (KC_s)C]^m} \tag{1}$$

With the assumption of constant diffusivity, a mass balance for the reactant in a catalyst pellet yields

$$D_e \nabla^2 C = r(C) \tag{2}$$

Extending previous results published by Aris (1957), Knudsen et al (1966) showed that the correlations of effectiveness factor and Thiele modulus for a sphere, cylinder, and flat plate lie close together when the characteristic dimension in the Thiele modulus is defined as the ratio of the volume to the outside surface through which the reactant can diffuse. Therefore, a simplified analysis for a flat plate can be extended to catalyst pellets of dif-

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